Reprinted from *The Journal of Chemical Physics*,
Vol. 40, No. 8, pp. 2309–2325, April 15, 1964

18p

N64-25508

Code none
NASA CR56782

Cat 20

Technical Report No. 32-549

Zero-Field Splitting, One- and Two-Center Coulomb-Type Integrals

Murray Geller
Richard W. Griffith

001

This paper presents the results of one phase of research carried out at the Jet Propulsion Laboratory, California Institute of Technology, under Contract No. NAS 7-100, sponsored by the National Aeronautics and Space Administration.

JET PROPULSION LABORATORY
CALIFORNIA INSTITUTE OF TECHNOLOGY
PASADENA, CALIFORNIA

April 15, 1964

Reprinted from THE JOURNAL OF CHEMICAL PHYSICS, Vol. 40, No. 8, 2309–2325, 15 April 1964
Printed in U. S. A.

Zero-Field Splitting, One- and Two-Center Coulomb-Type Integrals*

MURRAY GELLER AND RICHARD W. GRIFFITH†
Jet Propulsion Laboratory, 4800 Oak Grove Drive, Pasadena, California

25508

(Received 31 October 1963)

One- and two-center Coulomb-type integrals of the form

$$\int [N, L, M]_{a1} O_{1,2} [N', L', M']_{b2} d\tau_1 d\tau_2,$$

where O_1 and O_2 are the two-particle operators $\frac{1}{2}r_{12}^{-5}(3z_{12}^2-r_{12}^2)$ and $3r_{12}^{-5}(x_{12}^2-y_{12}^2)$, respectively, needed in the evaluation of zero-field splitting, are evaluated in closed analytical form.

Author

I. INTRODUCTION

THERE has been much concern recently over the origin and calculation of the three component levels of a triplet state in a molecule even when no external fields are present.[1–8] It is now clear that this zero-field splitting of the spin multiplet is a manifestation of pure spin–spin interaction and can be represented by the Hamiltonian[9] term

$$H' = g^2\beta^2 \sum_{i<j} \left\{ \frac{\mathbf{s}_i \cdot \mathbf{s}_j}{r_{ij}^3} - 3\frac{(\mathbf{s}_i \cdot \mathbf{r}_{ij})(\mathbf{s}_j \cdot \mathbf{r}_{ij})}{r_{ij}^5} \right\}, \qquad (1)$$

where g is the gyromagnetic ratio, β is the Bohr magneton, $\mathbf{s}_i$ is the spin vector of the ith electron (in units of $\hbar$), and $\mathbf{r}_{ij}$ is the position vector connecting electrons i and j.

To obtain the matrix elements of H' over a basis consisting of general atomic orbitals (AO's) on Atom a, χ_a, χ_a', and AO's on Atom b, χ_b, χ_b', we can reduce the calculation to the evaluation of the following two types of two-center Coulomb-type integrals[10] (see Fig. 1 for

* Supported by NASA Contract No. NAS 7-100.
† Present address: Department of Physics, California Institute of Technology, Pasadena, California.
[1] M. Tinkham and M. P. Strandberg, Phys. Rev. **97**, 937 (1955).
[2] C. A. Hutchinson, Jr., and B. W. Mangum, J. Chem. Phys. **29**, 952 (1958); **32**, 1261 (1960); **34**, 908 (1961).
[3] M. Gouterman and W. Moffitt, J. Chem. Phys. **30**, 1107 (1957); M. Gouterman, J. Chem. Phys. **30**, 1369 (1959).
[4] H. F. Hameka, J. Chem. Phys. **31**, 315 (1959); R. M. Pitzer and H. F. Hameka, *ibid.* **37**, 2725 (1962).
[5] R. McWeeny, J. Chem. Phys. **34**, 399, 1065 (1961).
[6] P. R. Fontana, Phys. Rev. **125**, 220 (1962).
[7] J. Higuchi, J. Chem. Phys. **38**, 1237 (1963).
[8] R. D. Sharma, J. Chem. Phys. **38**, 2350 (1963).
[9] A. D. MacLachlan, Mol. Phys. **6**, 441 (1963); H. A. Bethe and E. E. Salpeter *Quantum Mechanics of One- and Two-Electron Atoms* (Academic Press Inc., New York, 1957), p. 181.
[10] Two-center exchange type integrals also appear, but as they cannot be evaluated by the methods of this paper, they will be ignored for the present.

TABLE I. Transforms of $[N, L, M]$ for $N=1, 2, 3$.

$$[1S]^{\mathrm{T}}=p^4(k^2+p^2)^{-2}$$

$$[2S]^{\mathrm{T}}=(1/3)p^4[4p^2(k^2+p^2)^{-3}-(k^2+p^2)^{-2}]$$

$$\left.\begin{matrix}[2P\Sigma]^{\mathrm{T}}\\ [2P\Pi]^{\mathrm{T}}\\ [2P]\bar{\Pi}^{\mathrm{T}}\end{matrix}\right\}=2ikp^5(k^2+p^2)^{-3}\left\{\begin{matrix}P_1(\cos u)\\ P_1^1(\cos u)\cos v\\ P_1^1(\cos u)\sin v\end{matrix}\right.$$

$$[3S]^{\mathrm{T}}=p^6[2p^2(k^2+p^2)^{-4}-(k^2+p^2)^{-3}]$$

$$\left.\begin{matrix}[3P\Sigma]^{\mathrm{T}}\\ [3P\Pi]^{\mathrm{T}}\\ [3P\bar{\Pi}]^{\mathrm{T}}\end{matrix}\right\}=(2/5)ikp^5[6p^2(k^2+p^2)^{-4}-(k^2+p^2)^{-3}]\left\{\begin{matrix}P_1(\cos u)\\ P_1^1(\cos u)\cos v\\ P_1^1(\cos u)\sin v\end{matrix}\right.$$

$$\left.\begin{matrix}[3D\Sigma]^{\mathrm{T}}\\ [3D\Pi]^{\mathrm{T}}\\ [3D\bar{\Pi}]^{\mathrm{T}}\\ [3D\Delta]^{\mathrm{T}}\\ [3D\bar{\Delta}]^{\mathrm{T}}\end{matrix}\right\}=(2/9)\sqrt{3}p^6[p^2(k^2+p^2)^{-4}-(k^2+p^2]^{-3}]\left\{\begin{matrix}2\sqrt{3}P_2(\cos u)\\ 2P_2^1(\cos u)\cos v\\ 2P_2^1(\cos u)\sin v\\ P_2^2(\cos u)\cos 2v\\ P_2^2(\cos u)\sin 2v\end{matrix}\right.$$

the appropriate notation):

$$l_1=\int\chi_a(1)\chi_a'(1)O_1\chi_b(2)\chi_b'(2)d\tau_1d\tau_2;$$

$$l_2=\int\chi_a(1)\chi_a'(1)O_2\chi_b(2)\chi_b'(2)d\tau_1d\tau_2, \qquad (2)$$

where O_1 and O_2 are the following two-particle operators

$$O_1=\tfrac{1}{2}r_{12}^{-5}(3z_{12}^2-r_{12}^2)=r_{12}^{-3}P_2(\cos\theta_{12});$$

$$O_2=3r_{12}^{-5}(x_{12}^2-y_{12}^2)=r_{12}^{-3}P_2^2(\cos\theta_{12})\cos 2\phi_{12}. \qquad (3)$$

In what follows, we consider all the possibilities that arise from the use of Slater AO's with arbitrary values for the effective nuclear charges and with principal quantum numbers 1 and 2. All these integrals for the two-center case (as well as the one-center case) are obtained in closed analytical form here. Other authors have attempted to approximate these integrals by using Gaussian AO's[3] or point charge formulas[4,5] in the two-center cases, and only special one-center cases[4,8,11] have been done analytically, but to the author's knowledge, no systematic study is available.

[11] R. M. Pitzer, C. W. Kern, and W. N. Lipscomb, J. Chem. Phys. **37**, 267 (1962).

II. CHOICE OF ORBITALS AND METHOD OF EVALUATION

We adhere as closely as possible to the notation, choice of AO's, units, and coordinate system as used by Roothaan.[12] Rather than using Slater atomic orbitals (n, l, m) directly in the evaluation of the integrals of Eq. (2), we evaluate the integrals l_1 and l_2 over basic charge distributions[12] $[N, L, M]$.

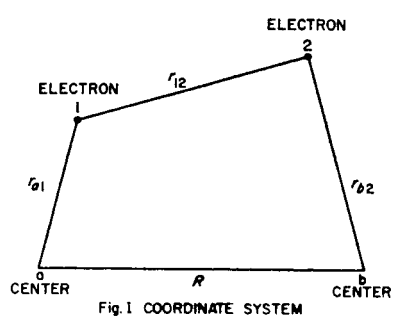

FIG. 1. Coordinate system.

[12] C. C. J. Roothaan, J. Chem. Phys. **19**, 1445 (1951).

TABLE II. Integrals I_1 over auxiliary functions A and B.

$$[1S_a \mid 1 \mid 1S_b] = (2/3)\,\pi^{-1}p_a^4p_b^4A(2;2,2)$$

$$[1S_a \mid 1 \mid 2S_b] = (2/9)\,\pi^{-1}p_a^4p_b^4[4p_b^2A(2;2,3) - A(2;2,2)]$$

$$[1S_a \mid 1 \mid 3S_b] = (2/3)\,\pi^{-1}p_a^4p_b^6[2p_b^2A(2;2,4) - A(2;2,3)]$$

$$[2S_a \mid 1 \mid 2S_b] = (2/27)\,\pi^{-1}p_a^4p_b^4[16p_a^2p_b^2A(2;3,3) - 4p_a^2(2;3,2) - 4p_b^2A(2;2,3) + A(2;2,2)]$$

$$[2S_a \mid 1 \mid 3S_b] = (2/9)\,\pi^{-1}p_a^4p_b^6[8p_a^2p_b^2A(2;3,4) - 4p_a^2A(2;3,3) - 2p_b^2A(2;2,4) + A(2;2,3)]$$

$$[3S_a \mid 1 \mid 3S_b] = (2/3)\,\pi^{-1}p_a^6p_b^6[4p_a^2p_b^2A(2;4,4) - 2p_a^2A(2;4,3) - 2p_b^2A(2;3,4) + A(2;3,3)]$$

$$[1S_a \mid 1 \mid 2P\Sigma_b] = (4/15)\,\pi^{-1}p_a^4p_b^5[3B(3;2,3) - 2B(1;2,3)]$$

$$[1S_a \mid 1 \mid 3P\Sigma_b] = (4/75)\,\pi^{-1}p_a^4p_b^5[18p_b^2B(3;2,4) - 3B(3;2,3) - 12p_b^2B(1;2,4) + 2B(1;2,3)]$$

$$[2S_a \mid 1 \mid 2P\Sigma_b] = (4/45)\,\pi^{-1}p_a^4p_b^5[12p_a^2B(3;3,3) - 3B(3;2,3) - 8p_a^2B(1;3,3) + 2B(1;2,3)]$$

$$\begin{aligned}[2S_a \mid 1 \mid 3P\Sigma_b] = (4/225)\,\pi^{-1}p_a^4p_b^5[&72p_a^2p_b^2B(3;3,4) - 12p_a^2B(3;3,3) - 18p_b^2B(3;2,4) + 3B(3;2,3)\\ &-48p_a^2p_b^2B(1;3,4) + 8p_a^2B(1;3,3) + 12p_b^2B(1;2,4) - 2B(1;2,3)]\end{aligned}$$

$$[3S_a \mid 1 \mid 2P\Sigma_b] = (4/15)\,\pi^{-1}p_a^6p_b^5[6p_a^2B(3;4,3) - 3B(3;3,3) - 4p_a^2B(1;4,3) + 2B(1;3,3)]$$

$$\begin{aligned}[3S_a \mid 1 \mid 3P\Sigma_b] = (4/75)\,\pi^{-1}p_a^6p_b^5[&36p_a^2p_b^2B(3;4,4) - 6p_a^2B(3;4,3) - 18p_b^2B(3;3,4) + 3B(3;3,3)\\ &-24p_a^2p_b^2B(1;4,4) + 4p_a^2B(1;4,3) + 12p_b^2B(1;3,4) - 2B(1;3,3)]\end{aligned}$$

$$\begin{aligned}[1S_a \mid 1 \mid 3D\Sigma_b] = -(8/9)\,\pi^{-1}p_a^4p_b^6[&(18/35)\{p_b^2A(4;2,4) - A(4;2,3)\} - (2/7)\{p_b^2A(2;2,4) - A(2;2,3)\}\\ &+(1/5)\{p_b^2A(0;2,4) - A(0;2,3)\}]\end{aligned}$$

$$\begin{aligned}[2S_a \mid 1 \mid 3D\Sigma_b] = -(8/27)\,\pi^{-1}p_a^4p_b^6[&(18/35)\{4p_a^2p_b^2A(4;3,4) - 4p_a^2A(4;3,3) - p_b^2A(4;2,4) + A(4;2,3)\}\\ &-(2/7)\{4p_a^2p_b^2A(2;3,4) - 4p_a^2A(2;3,3) - p_b^2A(2;2,4) + A(2;2,3)\}\\ &+(1/5)\{4p_a^2p_b^2A(0;3,4) - 4p_a^2A(0;3,3) - p_b^2A(0;2,4) + A(0;2,3)\}]\end{aligned}$$

$$\begin{aligned}[3S_a \mid 1 \mid 3D\Sigma_b] = -(8/9)\,\pi^{-1}p_a^6p_b^6[&(18/35)\{2p_a^2p_b^2A(4;4,4) - 2p_a^2A(4;4,3) - p_b^2A(4;3,4) + A(4;3,3)\}\\ &-(2/7)\{2p_a^2p_b^2A(2;4,4) - 2p_a^2A(2;4,3) - p_b^2A(2;3,4) + A(2;3,3)\}\\ &+(1/5)\{2p_a^2p_b^2A(0;4,4) - 2p_a^2A(0;4,3) - p_b^2A(0;3,4) + A(0;3,3)\}]\end{aligned}$$

$$\begin{aligned}[2P\Sigma_a \mid 1 \mid 2P\Sigma_b] = -(8/3)\,\pi^{-1}p_a^5p_b^5[&(12/35)\{p_a^2A(4;3,3) - A(4;2,3)\} - (11/21)\{p_a^2A(2;3,3) - A(2;2,3)\}\\ &+(2/15)\{p_a^2A(0;3,3) - A(0;2,3)\}]\end{aligned}$$

$$\begin{aligned}[2P\Sigma_a \mid 1 \mid 3P\Sigma_b] = -(8/15)\,\pi^{-1}p_a^5p_b^5[&(12/35)\{6p_b^4A(4;3,4) - 7p_b^2A(4;3,3) + A(4;3,2)\}\\ &-(11/21)\{6p_b^4A(2;3,4) - 7p_b^2A(2;3,3) + A(2;3,2)\}\\ &+(2/15)\{6p_b^4A(0;3,4) - 7p_b^2A(\mathrm{O};3,3) + A(0;3,2)\}]\end{aligned}$$

$$\begin{aligned}[3P\Sigma_a \mid 1 \mid 3P\Sigma_b] = -(8/75)\,\pi^{-1}p_a^5p_b^5[&(12/35)\{36p_a^2p_b^4A(4;4,4) - 42p_a^2p_b^2A(4;4,3)\\ &+6p_a^2A(4;4,2) - 6p_b^4A(4;3,4) + 7p_b^2A(4;3,3) - A(4;3,2)\}\\ &-(11/21)\{36p_a^2p_b^4A(2;4,4) - 42p_a^2p_b^2A(2;4,3) + 6p_a^2A(2;4,2) - 6p_b^4A(2;3,4)\\ &+7p_b^2A(2;3,3) - A(2;3,2)\} + (2/15)\{36p_a^2p_b^4A(0;4,4) - 42p_a^2p_b^2A(0;4,3)\\ &+6p_a^2A(0;4,2) - 6p_b^4A(0;3,4) + 7p_b^2A(0;3,3) - A(0;3,2)\}]\end{aligned}$$

$$\begin{aligned}[2P\Sigma_a \mid 1 \mid 3D\Sigma_b] = -(16/9)\,\pi^{-1}p_a^5p_b^6[&(2/7)\{p_b^2B(5;3,4) - B(5;3,3)\} - (2/5)\{p_b^2B(3;3,4) - B(3;3,3)\}\\ &+(11/35)\{p_b^2B(1;3,4) - B(1;3,3)\}]\end{aligned}$$

TABLE II (*Continued*)

$$[3P\Sigma_a \mid 1 \mid 3D\Sigma_b] = -(16/45)\,\pi^{-1}p_a^5p_b^6[(2/7)\{6p_a^2p_b^2B(5;4,4)-6p_a^2B(5;4,3)-p_b^2B(5;3,4)+B(5;3,3)\}$$
$$-(2/5)\{6p_a^2p_b^2B(3;4,4)-6p_a^2B(3;4,3)-p_b^2B(3;3,4)+B(3;3,3)\}$$
$$+(11/35)\{6p_a^2p_b^2B(1;4,4)-6p_a^2B(1;4,3)-p_b^2B(1;3,4)+B(1;3,3)\}]$$

$$[3D\Sigma_a \mid 1 \mid 3D\Sigma_b] = (32/27)\,\pi^{-1}p_a^6p_b^6[(18/77)\{p_a^2p_b^2A(6;4,4)-p_a^2A(6;4,3)-p_b^2A(6;3,4)+A(6;3,3)\}$$
$$-(108/385)\{p_a^2p_b^2A(4;4,4)-p_a^2A(4;4,3)-p_b^2A(4;3,4)+A(4;3,3)\}$$
$$+(3/7)\{p_a^2p_b^2A(2;4,4)-p_a^2A(2;4,3)-p_b^2A(2;3,4)+A(2;3,3)\}$$
$$-(2/35)\{p_a^2p_b^2A(0;4,4)-p_a^2A(0;4,3)-p_b^2A(0;3,4)+A(0;3,3)\}]$$

$$[2P\Pi_a \mid 1 \mid 2P\Pi_b] = (4/3)\,\pi^{-1}p_a^5p_b^5[(12/35)\{p_a^2A(4;3,3)-A(4;2,3)\}+(10/21)\{p_a^2A(2;3,3)-A(2;2,3)\}$$
$$+(2/15)\{p_a^2A(0;3,3)-A(0;2,3)\}$$
$$=[2P\bar{\Pi}_a \mid 1 \mid 2P\bar{\Pi}_b]$$

$$[2P\Pi_a \mid 1 \mid 3P\Pi_b] = (4/15)\,\pi^{-1}p_a^5p_b^5[(12/35)\{6p_b^4A(4;3,4)-7p_b^2A(4;3,3)+A(4;3,2)\}$$
$$+(10/21)\{6p_b^4A(2;3,4)-7p_b^2A(2;3,3)+A(2;3,2)\}$$
$$+(2/15)\{6p_b^4A(0;3,4)-7p_b^2A(0;3,3)+A(0;3,2)\}]$$
$$=[2P\bar{\Pi}_a \mid 1 \mid 3P\bar{\Pi}_b]$$

$$[3P\Pi_a \mid 1 \mid 3P\Pi_b] = (4/75)\,\pi^{-1}p_a^5p_b^5[(12/35)\{36p_a^2p_b^4A(4;4,4)-42p_a^2p_b^2A(4;4,3)$$
$$+6p_a^2A(4;4,2)-6p_b^4A(4;3,4)+7p_b^2A(4;3,3)-A(4;3,2)\}$$
$$+(10/21)\{36p_a^2p_b^4A(2;4,4)-42p_a^2p_b^2A(2;4,3)+6p_a^2A(2;4,2)-6p_b^4A(2;3,4)$$
$$+7p_b^2A(2;3,3)-A(2;3,2)\}+(2/15)\{36p_a^2p_b^4A(0;4,4)-42p_a^2p_b^2A(0;4,3)$$
$$+6p_a^2A(0;4,2)-6p_b^4A(0;3,4)+7p_b^2A(0;3,3)-A(0;3,2)\}]$$
$$=[3P\bar{\Pi}_a \mid 1 \mid 3P\bar{\Pi}_b]$$

$$[2P\Pi_a \mid 1 \mid 3D\Pi_b] = (8/27)\sqrt{3}\,\pi^{-1}p_a^5p_b^6[(4/7)\{p_b^2B(5;3,4)-B(5;3,3)\}+(2/5)\{p_b^2B(3;3,4)-B(3;3,3)\}$$
$$-(6/35)\{p_b^2B(1;3,4)-B(1;3,3)\}]$$
$$=[2P\bar{\Pi}_a \mid 1 \mid 3D\bar{\Pi}_b]$$

$$[3P\Pi_a \mid 1 \mid 3D\Pi_b] = (8/135)\sqrt{3}\,\pi^{-1}p_a^5p_b^6[(4/7)\{6p_a^2p_b^2B(5;4,4)-6p_a^2B(5;4,3)-p_b^2B(5;3,4)+B(5;3,3)\}$$
$$+(2/5)\{6p_a^2p_b^2B(3;4,4)-6p_a^2B(3;4,3)-p_b^2B(3;3,4)+B(3;3,3)\}$$
$$-(6/35)\{6p_a^2p_b^2B(1;4,4)-6p_a^2B(1;4,3)-p_b^2B(1;3,4)+B(1;3,3)\}]$$
$$=[3P\bar{\Pi}_a \mid 1 \mid 3D\bar{\Pi}_b]$$

$$[3D\Pi_a \mid 1 \mid 3D\Pi_b] = -(16/81)\,\pi^{-1}p_a^6p_b^6[(72/77)\{p_a^2p_b^2A(6;4,4)-p_a^2A(6;4,3)-p_b^2A(6;3,4)+A(6;3,3)\}$$
$$-(36/385)\{p_a^2p_b^2A(4;4,4)-p_a^2A(4;4,3)-p_b^2A(4;3,4)+A(4;3,3)\}$$
$$-(6/7)\{p_a^2p_b^2A(2;4,4)-p_a^2A(2;4,3)-p_b^2A(2;3,4)+A(2;3,3)\}$$
$$+(6/35)\{p_a^2p_b^2A(0;4,4)-p_a^2A(0;4,3)-p_b^2A(0;3,4)+A(0;3,3)\}]$$
$$=[3D\bar{\Pi}_a \mid 1 \mid 3D\bar{\Pi}_b]$$

$$[3D\Delta_a \mid 1 \mid 3D\Delta_b] = (4/81)\,\pi^{-1}p_a^6p_b^6[(72/77)\{p_a^2p_b^2A(6;4,4)-p_a^2A(6;4,3)-p_b^2A(6;3,4)+A(6;3,3)\}$$
$$+(1152/385)\{p_a^2p_b^2A(4;4,4)-p_a^2A(4;4,3)-p_b^2A(4;3,4)+A(4;3,3)\}$$
$$+(24/7)\{p_a^2p_b^2A(2;4,4)-p_a^2A(2;4,3)-p_b^2A(2;3,4)+A(2;3,3)\}$$
$$+(48/35)\{p_a^2p_b^2A(0;4,4)-p_a^2A(0;4,3)-p_b^2A(0;3,4)+A(0;3,3)\}]$$
$$=[3D\bar{\Delta}_a \mid 1 \mid 3D\bar{\Delta}_b]$$

TABLE III. Integrals I_2 over auxiliary functions A and B.

$$[1S_a \mid 2 \mid 3D\Delta_b) = -(1/27)\sqrt{3}\,\pi^{-1}p_a^4p_b^6[(144/35)\{p_b^2A(4;2,4)-A(4;2,3)\} + (96/7)\{p_b^2A(2;2,4)-A(2;2,3)\}+(48/5)\{p_b^2A(0;2,4)-A(0;2,3)\}]$$

$$[2S_a \mid 2 \mid 3D\Delta_b] = -(1/81)\sqrt{3}\,\pi^{-1}p_a^4p_b^6[(144/35)\{4p_a^2p_b^2A(4;3,4)-4p_a^2A(4;3,3) -p_b^2A(4;2,4)+A(4;2,3)\}+(96/7)\{4p_a^2p_b^2A(2;3,4)-4p_a^2A(2;3,3) -p_b^2A(2;2,4)+A(2;2,3)\}+(48/5)\{4p_a^2p_b^2A(0;3,4)-4p_a^2A(0;3,3) -p_b^2A(0;2,4)+A(0;2,3)\}]$$

$$[3S_a \mid 2 \mid 3D\Delta_b] = -(1/27)\sqrt{3}\,\pi^{-1}p_a^6p_b^6[(144/35)\{2p_a^2p_b^2A(4;4,4)-2p_a^2A(4;4,3)-p_b^2A(4;3,4) +A(4;3,3)\}+(96/7)\{2p_a^2p_b^2A(2;4,4)-2p_a^2A(2;4,3)-p_b^2A(2;3,4)+A(2;3,3)\} +(48/5)\{2p_a^2p_b^2A(0;4,4)-2p_a^2A(0;4,3)-p_b^2A(0;3,4)+A(0;3,3)\}]$$

$$[2P\Pi_a \mid 2 \mid 2P\Pi_b] = -(1/3)\,\pi^{-1}p_a^5p_b^5[(48/35)\{p_a^2A(4;3,3)-A(4;2,3)\} +(32/7)\{p_a^2A(2;3,3)-A(2;2,3)\}+(16/5)\{p_a^2A(0;3,3)-A(0;2,3)\}] = -[2P\bar{\Pi}_a \mid 2 \mid 2P\bar{\Pi}_b]$$

$$[2P\Pi_a \mid 2 \mid 3P\Pi_b] = -(1/15)\,\pi^{-1}p_a^5p_b^5[(48/35)\{6p_b^4A(4;3,4)-7p_b^2A(4;3,3)+A(4;3,2)\} +(32/7)\{6p_b^4A(2;3,4)-7p_b^2A(2;3,3)+A(2;3,2)\} +(16/5)\{6p_b^4A(0;3,4)-7p_b^2A(0;3,3)+A(0;3,2)\}] = -[2P\bar{\Pi}_a \mid 2 \mid 3P\bar{\Pi}_b]$$

$$[3P\Pi_a \mid 2 \mid 3P\Pi_b] = -(1/75)\,\pi^{-1}p_a^5p_b^5[(48/35)\{36p_a^2p_b^4A(4;4,4)-42p_a^2p_b^2A(4;4,3)+6p_a^2A(4;4,2) -6p_b^4A(4;3,4)+7p_b^2A(4;3,3)-A(4;3,2)\}+(32/7)\{36p_a^2p_b^4A(2;4,4) -42p_a^2p_b^2A(2;4,3)+6p_a^2A(2;4,2)-6p_b^4A(2;3,4)+7p_b^2A(2;3,3)-A(2;3,2)\} +(16/5)\{36p_a^2p_b^4A(0;4,4)-42p_a^2p_b^2A(0;4,3)+6p_a^2A(0;4,2)-6p_b^4A(0;3,4) +7p_b^2A(0;3,3)-A(0;3,2)\}] = -[3P\bar{\Pi}_a \mid 2 \mid 3P\bar{\Pi}_b]$$

$$[2P\Pi_a \mid 2 \mid 3D\Pi_b] = -(2/27)\sqrt{3}\,\pi^{-1}p_a^5p_b^6[(16/7)\{p_b^2B(5;3,4)-B(5;3,3)\}+(32/5)\{p_b^2B(3;3,4)-B(3;3,3)\} +(144/35)\{p_b^2B(1;3,4)-B(1;3,3)\}] = -[2P\bar{\Pi}_a \mid 2 \mid 3D\bar{\Pi}_b]$$

$$[3P\Pi_a \mid 2 \mid 3D\Pi_b] = -(2/135)\sqrt{3}\,\pi^{-1}p_a^5p_b^6[(16/7)\{6p_a^2p_b^2B(5;4,4)-6p_a^2B(5;4,3) -p_b^2B(5;3,4)+B(5;3,3)\}+(32/5)\{6p_a^2p_b^2B(3;4,4)-6p_a^2B(3;4,3) -p_b^2B(3;3,4)+B(3;3,3)\}+(144/35)\{6p_a^2p_b^2B(1;4,4)-6p_a^2B(1;4,3) -p_b^2B(1;3,4)+B(1;3,3)\}] = -[3P\bar{\Pi}_a \mid 2 \mid 3D\bar{\Pi}_b]$$

$$[3D\Pi_a \mid 2 \mid 3D\Pi_b] = (4/81)\,\pi^{-1}p_a^6p_b^6[(288/77)\{p_a^2p_b^2A(6;4,4)-p_a^2A(6;4,3)-p_b^2A(6;3,4)+A(6;3,3)\} +(432/55)\{p_a^2p_b^2A(4;4,4)-p_a^2A(4;4,3)-p_b^2A(4;3,4)+A(4;3,3)\} -(144/35)\{p_a^2p_b^2A(0;4,4)-p_a^2A(0;4,3)-p_b^2A(0;3,4)+A(0;3,3)\}] = -[3D\bar{\Pi}_a \mid 2 \mid 3D\bar{\Pi}_b]$$

$$[2P\Sigma_a \mid 2 \mid 3D\Delta_b] = -(2/27)\sqrt{3}\,\pi^{-1}p_a^5p_b^6[(16/7)\{p_b^2B(5;3,4)-B(5;3,3)\} +(32/5)\{p_b^2B(3;3,4)-B(3;3,3)\}+(144/35)\{p_b^2B(1;3,4)-B(1;3,3)\}]$$

$$[3P\Sigma_a \mid 2 \mid 3D\Delta_b] = -(2/135)\sqrt{3}\,\pi^{-1}p_a^5p_b^6[(16/7)\{6p_a^2p_b^2B(5;4,4)-6p_a^2B(5;4,3)-p_b^2B(5;3,4)+B(5;3,3)\} +(32/5)\{6p_a^2p_b^2B(3;4,4)-6p_a^2B(3;4,3)-p_b^2B(3;3,4)+B(3;3,3)\} +(144/35)\{6p_a^2p_b^2B(1;4,4)-6p_a^2B(1;4,3)-p_b^2B(1;3,4)+B(1;3,3)\}]$$

$$[3D\Sigma_a \mid 2 \mid 3D\Delta_b] = (4/81)\sqrt{3}\,\pi^{-1}p_a^6p_b^6[(144/77)\{p_a^2p_b^2A(6;4,4)-p_a^2A(6;4,3)-p_b^2A(6;3,4)+A(6;3,3)\} +(2304/385)\{p_a^2p_b^2A(4;4,4)-p_a^2A(4;4,3)-p_b^2A(4;3,4)+A(4;3,3)\} +(48/7)\{p_a^2p_b^2A(2;4,4)-p_a^2A(2;4,3)-p_b^2A(2;3,4)+A(2;3,3)\} +(96/35)\{p_a^2p_b^2A(0;4,4)-p_a^2A(0;4,3)-p_b^2A(0;3,4)+A(0;3,3)\}]$$

TABLE IV. Expressions for the $F_n(\gamma)$ of Eq. (20) for $n=0, 1, 2, \cdots, 7$.

$$F_0(\gamma)=\gamma^{-1}-\gamma^{-1}e^{-\gamma}$$

$$F_1(\gamma)=[\gamma^{-1}-(2/\gamma^3)]+(2/\gamma^2)(1+\gamma^{-1})e^{-\gamma}$$

$$F_2(\gamma)=\left(\gamma^{-1}-\frac{4}{\gamma^3}+\frac{24}{\gamma^5}\right)-\frac{2^2\cdot 2!}{\gamma^3}\left(1+\frac{3}{\gamma}+\frac{3}{\gamma^2}\right)e^{-\gamma}$$

$$F_3(\gamma)=\left(\gamma^{-1}-\frac{6}{\gamma^3}+\frac{72}{\gamma^5}-\frac{720}{\gamma^7}\right)+\frac{2^3\cdot 3!}{\gamma^4}\left(1+\frac{6}{\gamma}+\frac{15}{\gamma^2}+\frac{15}{\gamma^3}\right)e^{-\gamma}$$

$$F_4(\gamma)=\left(\gamma^{-1}-\frac{8}{\gamma^3}+\frac{144}{\gamma^5}-\frac{2880}{\gamma^7}+\frac{40\,320}{\gamma^9}\right)-\frac{2^4\cdot 4!}{\gamma^5}\left(1+\frac{10}{\gamma}+\frac{45}{\gamma^2}+\frac{105}{\gamma^3}+\frac{105}{\gamma^4}\right)e^{-\gamma}$$

$$F_5(\gamma)=\left(\gamma^{-1}-\frac{10}{\gamma^3}+\frac{240}{\gamma^5}-\frac{7200}{\gamma^7}+\frac{201\,600}{\gamma^9}-\frac{3\,628\,800}{\gamma^{11}}\right)+\frac{2^5\cdot 5!}{\gamma^6}\left(1+\frac{15}{\gamma}+\frac{105}{\gamma^2}+\frac{420}{\gamma^3}+\frac{945}{\gamma^4}+\frac{945}{\gamma^5}\right)e^{-\gamma}$$

$$F_6(\gamma)=\left(\gamma^{-1}-\frac{12}{\gamma^3}+\frac{360}{\gamma^5}-\frac{14\,400}{\gamma^7}+\frac{604\,800}{\gamma^9}-\frac{21\,772\,800}{\gamma^{11}}+\frac{479\,001\,600}{\gamma^{13}}\right)$$
$$-\frac{2^6\cdot 6!}{\gamma^7}\left(1+\frac{21}{\gamma}+\frac{210}{\gamma^2}+\frac{1260}{\gamma^3}+\frac{4725}{\gamma^4}+\frac{10\,395}{\gamma^5}+\frac{10\,395}{\gamma^6}\right)e^{-\gamma}$$

$$F_7(\gamma)=\left(\gamma^{-1}-\frac{14}{\gamma^3}+\frac{504}{\gamma^5}-\frac{25\,200}{\gamma^7}+\frac{1\,411\,200}{\gamma^9}-\frac{21\cdot 10!}{\gamma^{11}}+\frac{7\cdot 12!}{\gamma^{13}}-\frac{14!}{\gamma^{15}}\right)$$
$$+\frac{2^7\cdot 7!}{\gamma^8}\left(1+\frac{28}{\gamma}+\frac{378}{\gamma^2}+\frac{3150}{\gamma^3}+\frac{17\,325}{\gamma^4}+\frac{62\,370}{\gamma^5}+\frac{135\,135}{\gamma^6}+\frac{135\,135}{\gamma^7}\right)e^{-\gamma}$$

If (n, l, m) is a Slater orbital

$$(n, l, m)=(2\zeta)^{n+\frac{1}{2}}[(2n)!]^{-\frac{1}{2}}r^{n-1}\exp(-\zeta r)\,S_{l,m}(\theta, \phi), \tag{4}$$

where

$$S_{l,0}(\theta, \phi)=[(2l+1)/4\pi]^{\frac{1}{2}}P_l(\cos\theta),$$

and

$$S_{l,m}(\theta, \phi)=\left[\frac{2l+1}{2\pi}\,\frac{(l-|m|)!}{(l+|m|)!}\right]^{\frac{1}{2}}P_l^{|m|}(\cos\theta)\times\begin{Bmatrix}\cos|m|\phi\\ \sin|m|\phi\end{Bmatrix}, \tag{5}$$

then the product of two Slater orbitals with orbital exponents ζ_1 and ζ_2 on the same center can be decomposed to a sum of basic charge distributions $[N, L, M]$

$$[N, L, M]=[(2L+1)/4\pi]^{\frac{1}{2}}\times\{2^L(\zeta_1+\zeta_2)^{N+2}/(N+L+1)!\}r^{N-1}\times\exp[-[\zeta_1+\zeta_2]r)\,S_{L,M}(\theta, \phi). \tag{6}$$

For the cases involving the principal quantum numbers 1 and 2, all charge distributions up to $N=3$ arise. In analogy to the AO's, these basic charge distributions are denoted by NS, $NP\Sigma$, $NP\Pi$, $NP\bar{\Pi}$, $ND\Sigma$, $ND\Pi$, $ND\bar{\Pi}$, $ND\Delta$, and $ND\bar{\Delta}$. Roothaan gives explicit expressions[12] for the product of two Slater orbitals involving s and p electrons in terms of the basic charge distributions.

Thus, the integrals that are evaluated here are

$$I_1=\int[N, L, M]_{a1}O_1[N', L', M']_{b2}d\tau_1 d\tau_2$$
$$=[NLM_a\,|\,1\,|\,N'L'M_b']; \tag{7a}$$

$$I_2=\int[N, L, M]_{a1}O_2[N', L', M']_{b2}d\tau_1 d\tau_2$$
$$=[NLM_a\,|\,2\,|\,N'L'M_b']. \tag{7b}$$

The Fourier convolution method noted by Prosser and

TABLE V. $A(2m;\,1,\,1)$ and $B(2m+1;\,1,\,1)$ in terms of $F_n(\gamma)$ for different charges.

$$A(0;1,1)=+(1/2)\,\pi R(\beta^2-\alpha^2)^{-1}[\beta F_0(\beta)-\alpha F_0(\alpha)]$$
$$A(2;1,1)=-(2^3\cdot 2!)^{-1}\pi R(\beta^2-\alpha^2)^{-1}[\beta^3 F_2(\beta)-\alpha^3 F_2(\alpha)]$$
$$A(4;1,1)=+(2^5\cdot 4!)^{-1}\pi R(\beta^2-\alpha^2)^{-1}[\beta^5 F_4(\beta)-\alpha^5 F_4(\alpha)]$$
$$A(6;1,1)=-(2^7\cdot 6!)^{-1}\pi R(\beta^2-\alpha^2)^{-1}[\beta^7 F_6(\beta)-\alpha^7 F_6(\alpha)]$$
$$B(1;1,1)=-(2^2\cdot 1^1)^{-1}\pi(\beta^2-\alpha^2)^{-1}[\beta^3 F_1(\beta)-\alpha^3 F_1(\alpha)]$$
$$B(3;1,1)=+(2^4\cdot 3!)^{-1}\pi(\beta^2-\alpha^2)^{-1}[\beta^5 F_3(\beta)-\alpha^5 F_3(\alpha)]$$
$$B(5;1,1)=-(2^6\cdot 5!)^{-1}\pi(\beta^2-\alpha^2)^{-1}[\beta^7 F_5(\beta)-\alpha^7 F_5(\alpha)]$$

Blanchard[13] for one-electron two-center integrals, and used by one of the authors recently for one-electron two-center integrals over solid spherical harmonics[14] and for two-electron two-center integrals[15] is employed here. For the two-electron case, this method states that if we have the integral

$$J=\int f(\mathbf{r}_{a1})\,g(\mathbf{r}_{b2})\,h(\mathbf{r}_{12})\,d\tau_1 d\tau_2, \tag{8}$$

then the integral is recovered by

$$J=(2\pi)^{-3}\int f^{\mathrm{T}}(\mathbf{k})\,g^{\mathrm{T}}(\mathbf{k})\,h^{\mathrm{T}}(\mathbf{k})\,\exp(-i\mathbf{k}\cdot\mathbf{R})\,d\mathbf{k}, \tag{9}$$

where the superscript T indicates the appropriate Fourier transform,

$$\phi^{\mathrm{T}}(\mathbf{k})=\int \exp(i\mathbf{k}\cdot\mathbf{r})\,\phi(\mathbf{r})\,d\mathbf{r}, \tag{10}$$

TABLE VI. $A(2m;\,1,\,1)$ and $B(2m+1;\,1,\,1)$ in terms of $F_n(\gamma)$ for equal charges.

$$A(0;1,1)=+(2^3\cdot 1!)^{-1}\pi R\gamma^{-1}[\gamma^2 F_1(\gamma)+2F_0(\gamma)-\gamma]$$
$$A(2;1,1)=-(2^5\cdot 3!)^{-1}\pi R\gamma[\gamma^2 F_3(\gamma)+18F_2(\gamma)-\gamma]$$
$$A(4;1,1)=+(2^7\cdot 5!)^{-1}\pi R\gamma^3[\gamma^2 F_5(\gamma)+50F_4(\gamma)-\gamma]$$
$$A(6;1,1)=-(2^9\cdot 7!)^{-1}\pi R\gamma^5[\gamma^2 F_7(\gamma)+98F_6(\gamma)-\gamma]$$
$$B(1;1,1)=-(2^4\cdot 2!)^{-1}\pi\gamma[\gamma^2 F_2(\gamma)+12F_1(\gamma)-\gamma]$$
$$B(3;1,1)=+(2^6\cdot 4!)^{-1}\pi\gamma^3[\gamma^2 F_4(\gamma)+40F_3(\gamma)-\gamma]$$
$$B(5;1,1)=-(2^8\cdot 6!)^{-1}\pi\gamma^5[\gamma^2 F_6(\gamma)+84F_5(\gamma)-\gamma]$$

[13] F. P. Prosser and C. H. Blanchard, J. Chem. Phys. **36**, 1112 (1962).
[14] M. Geller, J. Chem. Phys. **39**, 84 (1963).
[15] M. Geller, J. Chem. Phys. **39**, 853 (1963).

k, u, and v are the spherical coordinates of the k vector, and R is the distance between the two centers a and b. In the one-center case ($R=0$), the integral is given by

$$J=(2\pi)^{-3}\int f^{\mathrm{T}}(\mathbf{k})\,g^{\mathrm{T}}(\mathbf{k})\,h^{\mathrm{T}}(\mathbf{k})\,d\mathbf{k}. \tag{11}$$

For further details concerning the evaluation of the transforms, the reader should consult Ref. 14.

III. RESULTING INTEGRALS OVER AUXILIARY FUNCTIONS

By the application of Eq. (9), we can write the integrals of Eq. (7) as

$$I_1=(2\pi)^{-3}\int[N,L,M]_{a1}{}^{\mathrm{T}}O_1{}^{\mathrm{T}}[N',L',M']_{b2}{}^{\mathrm{T}}\times\exp(-i\mathbf{k}\cdot\mathbf{R})\,d\mathbf{k}, \tag{12a}$$

$$I_2=(2\pi)^{-3}\int[N,L,M]_{a1}{}^{\mathrm{T}}O_2{}^{\mathrm{T}}[N',L',M']_{b2}{}^{\mathrm{T}}\times\exp(-i\mathbf{k}\cdot\mathbf{R})\,d\mathbf{k}. \tag{12b}$$

To evaluate Eqs. (12), we need the transforms of O_1, O_2 and of the $[N,L,M]$. From Eq. (11) of Ref. 14[16]

$$O_1{}^{\mathrm{T}}=-\tfrac{4}{3}\pi P_2(\cos u); \tag{13a}$$

$$O_2{}^{\mathrm{T}}=-\tfrac{4}{3}\pi P_2{}^2(\cos u)\cos 2v, \tag{13b}$$

and from Eq. (18) of Ref. 14:

$$[N,L,M]^{\mathrm{T}}=A\cdot\frac{P_L{}^{|m|}(\cos u)}{(k^2+p^2)^{N+1}}\begin{Bmatrix}\cos|M|v\\ \sin|M|v\end{Bmatrix}\times\sum_{s=0}^{s_0}(-1)^s\binom{N+L+1}{2s+2L+1}\frac{(s+L)!}{s!}\left(\frac{k}{p}\right)^{2s+L}, \tag{14}$$

[16] Reference 14 contains further details and definitions of all the quantities presented here.

TABLE VII. $k_m^p(\gamma)$ polynomials of Eqs. (26) for selected m and p values.

$$k_0^0(\gamma)=1$$

$$k_1^0(\gamma)=1+\gamma^{-1}$$

$$k_2^0(\gamma)=1+\frac{3}{\gamma}+\frac{3}{\gamma^2}$$

$$k_2^1(\gamma)=1+\frac{3}{\gamma}+\frac{6}{\gamma^2}+\frac{6}{\gamma^3}$$

$$k_2^2(\gamma)=1+\frac{4}{\gamma}+\frac{12}{\gamma^2}+\frac{24}{\gamma^3}+\frac{24}{\gamma^4}$$

$$k_2^3(\gamma)=1+\frac{6}{\gamma}+\frac{24}{\gamma^2}+\frac{72}{\gamma^3}+\frac{144}{\gamma^4}+\frac{144}{\gamma^5}$$

$$k_3^0(\gamma)=1+\frac{6}{\gamma}+\frac{15}{\gamma^2}+\frac{15}{\gamma^3}$$

$$k_3^1(\gamma)=1+\frac{5}{\gamma}+\frac{15}{\gamma^2}+\frac{30}{\gamma^3}+\frac{30}{\gamma^4}$$

$$k_3^2(\gamma)=1+\frac{5}{\gamma}+\frac{20}{\gamma^2}+\frac{60}{\gamma^3}+\frac{120}{\gamma^4}+\frac{120}{\gamma^5}$$

$$k_3^3(\gamma)\quad 1+\frac{6}{\gamma}+\frac{30}{\gamma^2}+\frac{120}{\gamma^3}+\frac{360}{\gamma^4}+\frac{720}{\gamma^5}+\frac{720}{\gamma^6}$$

$$k_4^0(\gamma)=1+\frac{10}{\gamma}+\frac{45}{\gamma^2}+\frac{105}{\gamma^3}+\frac{105}{\gamma^4}$$

$$k_4^1(\gamma)=1+\frac{10}{\gamma}+\frac{55}{\gamma^2}+\frac{195}{\gamma^3}+\frac{420}{\gamma^4}+\frac{420}{\gamma^5}$$

$$k_4^2(\gamma)=1+\frac{11}{\gamma}+\frac{75}{\gamma^2}+\frac{360}{\gamma^3}+\frac{1200}{\gamma^4}+\frac{2520}{\gamma^5}+\frac{2520}{\gamma^6}$$

$$k_4^3(\gamma)=1+\frac{13}{\gamma}+\frac{108}{\gamma^2}+\frac{660}{\gamma^3}+\frac{3000}{\gamma^4}+\frac{9720}{\gamma^5}+\frac{20\,160}{\gamma^6}+\frac{20\,160}{\gamma^7}$$

$$k_5^0(\gamma)=1+\frac{15}{\gamma}+\frac{105}{\gamma^2}+\frac{420}{\gamma^3}+\frac{945}{\gamma^4}+\frac{945}{\gamma^5}$$

$$k_5^1(\gamma)=1+\frac{14}{\gamma}+\frac{105}{\gamma^2}+\frac{525}{\gamma^3}+\frac{1785}{\gamma^4}+\frac{3780}{\gamma^5}+\frac{3780}{\gamma^6}$$

TABLE VII (*Continued*)

$$k_5^2(\gamma)=1+\frac{14}{\gamma}+\frac{119}{\gamma^2}+\frac{735}{\gamma^3}+\frac{3360}{\gamma^4}+\frac{10\,920}{\gamma^5}+\frac{22\,680}{\gamma^6}+\frac{22\,680}{\gamma^7}$$

$$k_5^3(\gamma)=1+\frac{15}{\gamma}+\frac{147}{\gamma^2}+\frac{1092}{\gamma^3}+\frac{6300}{\gamma^4}+\frac{27\,720}{\gamma^5}+\frac{88\,200}{\gamma^6}+\frac{181\,440}{\gamma^7}+\frac{181\,440}{\gamma^8}$$

$$k_6^0(\gamma)=1+\frac{21}{\gamma}+\frac{210}{\gamma^2}+\frac{1260}{\gamma^3}+\frac{4725}{\gamma^4}+\frac{10\,395}{\gamma^5}+\frac{10\,395}{\gamma^6}$$

$$k_6^1(\gamma)=1+\frac{21}{\gamma}+\frac{231}{\gamma^2}+\frac{1680}{\gamma^3}+\frac{8505}{\gamma^4}+\frac{29\,295}{\gamma^5}+\frac{62\,370}{\gamma^6}+\frac{62\,370}{\gamma^7}$$

$$k_6^2(\gamma)=1+\frac{22}{\gamma}+\frac{273}{\gamma^2}+\frac{2373}{\gamma^3}+\frac{15\,225}{\gamma^4}+\frac{71\,820}{\gamma^5}+\frac{238\,140}{\gamma^6}+\frac{498\,960}{\gamma^7}+\frac{498\,960}{\gamma^8}$$

$$k_6^3(\gamma)=1+\frac{24}{\gamma}+\frac{339}{\gamma^2}+\frac{3465}{\gamma^3}+\frac{27\,090}{\gamma^4}+\frac{163\,170}{\gamma^5}+\frac{740\,880}{\gamma^6}+\frac{2\,404\,080}{\gamma^7}+\frac{4\,989\,600}{\gamma^8}+\frac{4\,989\,600}{\gamma^9}$$

where

$$A=2^{2L+1}i^L p^{2N+2}[(2L)!]^{-1}\left[\binom{N+L+1}{2L+1}\right]^{-1}\times\left[\frac{(L-|M|)!}{(L+|M|)!}\right]^{\frac{1}{2}}[2(1+\delta_{m,0})]^{-\frac{1}{2}},$$

$$p=\zeta_1+\zeta_2,$$

and s_0 is the largest integer in $\frac{1}{2}(N-L)$. For convenience, Table I lists the specific transforms of $[N, L, M]$ for all cases through $N=3$.

The next phase in the evaluation of Eqs. (12) is the formation of all the products $[N, L, M]_{a1}{}^{\mathrm{T}}O_{1,2}{}^{\mathrm{T}}\times[N', L', M']_{b2}{}^{\mathrm{T}}$; e.g.,

$$[1S]_{a1}{}^{\mathrm{T}}O_2{}^{\mathrm{T}}[1S]_{b2}{}^{\mathrm{T}}=-\tfrac{4}{3}\pi p_a{}^4p_b{}^4(k^2+p_a{}^2)^{-2}\times(k^2+p_b{}^2)^{-2}P_2{}^2(\cos u)\cos 2v. \quad (15)$$

Once these products have been obtained, it is easy to derive the selection rules for I_1 and I_2:

(A) I_1 vanishes unless $M=M'$; thus the only remaining terms are those in which we have SS, $S\Sigma$, $\Sigma\Sigma$, $\Pi\Pi$, $\bar{\Pi}\bar{\Pi}$, $\Delta\Delta$, or $\bar{\Delta}\bar{\Delta}$.

(B) I_2 vanishes unless we have either $S\Delta$, $\Sigma\Delta$, $\Pi\Pi$, or $\bar{\Pi}\bar{\Pi}$.

Making use of the auxiliary functions

$$A(2m;p,q)=\int_0^\infty\frac{k^2j_{2m}(kR)\,dk}{(k^2+p_a{}^2)^p(k^2+p_b{}^2)^q}, \quad (16)$$

and

$$B(2m+1;p,q)=\int_0^\infty\frac{k^3j_{2m+1}(kR)\,dk}{(k^2+p_a{}^2)^p(k^2+p_b{}^2)^q}, \quad (17)$$

where $j_p(x)$ is a spherical Bessel function,[17] we can express all the nonvanishing integrals of Eqs. (7) (through $N=3$) in terms of the A and B auxiliary functions defined above. The results for I_1 are collected in Table II and the results for I_2 in Table III. From Tables II and III we see that all the integrals are expressible in terms of $A(2m;p,q)$, where $m=0$, 1, 2, and 3; and $B(2m+1;p,q)$ where $m=0$, 1, and 2; and p and q take on values up through $p=q=4$.

IV. EVALUATION OF AUXILIARY FUNCTIONS

The auxiliary functions $A(2m;p,q)$ and $B(2m+1;p,q)$ of Eqs. (16) and (17) can all be generated from the primitives $A(2m;1,1)$ and $B(2m+1;1,1)$ by the use of the following generating formulas:

$$A(2m;p+1,q+1)=(-\tfrac{1}{2}R^2)^{p+q}[p!q!]^{-1}\times[\alpha^{-1}(\partial/\partial\alpha)]^p[\beta^{-1}(\partial/\partial\beta)]^qA(2m;1,1); \quad (18)$$

[17] See A. Erdelyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vols. I, II for definitions and properties of all the special functions utilized here.

TABLE VIII. $A(2m;\,p,\,q)$ and $B(2m+1;\,p,\,q)$ in terms of $k_m{}^p(\gamma)$—case of different nuclear charges ($\alpha\neq\beta$).[a]

$$A(0;3,2)=-\pi R^7\Big[e^{-\beta}\{\tfrac{3}{2}[(\beta^2-\alpha^2)^4]^{-1}+(4\beta)^{-1}[(\beta^2-\alpha^2)^3]^{-1}\}$$
$$-e^{-\alpha}\Big\{\tfrac{3}{2}[(\beta^2-\alpha^2)^4]^{-1}-(2\alpha)^{-1}[(\beta^2-\alpha^2)^3]^{-1}+(16\alpha^2)^{-1}\frac{k_1{}^0(\alpha)}{(\beta^2-\alpha^2)^2}\Big\}\Big]$$

$$A(0;3,3)=-\pi R^9\Big[e^{-\beta}\Big\{3[(\beta^2-\alpha^2)^5]^{-1}+\frac{3}{4\beta}[(\beta^2-\alpha^2)^4]^{-1}+(16\beta^2)^{-1}\frac{k_1{}^0(\beta)}{(\beta^2-\alpha^2)^3}\Big\}$$
$$-e^{-\alpha}\Big\{3[(\beta^2-\alpha^2)^5]^{-1}-\frac{3}{4\alpha}[(\beta^2-\alpha^2)^4]^{-1}+(16\alpha^2)^{-1}\frac{k_1{}^0(\alpha)}{(\beta^2-\alpha^2)^3}\Big\}\Big]$$

$$A(0;4,2)=\pi R^9\Big[e^{-\beta}\{2[(\beta^2-\alpha^2)^5]^{-1}+(4\beta)^{-1}[(\beta^2-\alpha^2)^4]^{-1}\}$$
$$-e^{-\alpha}\Big\{2[(\beta^2-\alpha^2)^5]^{-1}-\frac{3}{4\alpha}[(\beta^2-\alpha^2)^4]^{-1}+(8\alpha^2)^{-1}\frac{k_1{}^0(\alpha)}{(\beta^2-\alpha^2)^3}-(96\alpha^3)^{-1}\frac{k_2{}^0(\alpha)}{(\beta^2-\alpha^2)^2}\Big\}\Big]$$

$$A(0;4,3)=\pi R^{11}\Big[e^{-\beta}\Big\{5[(\beta^2-\alpha^2)^6]^{-1}+(\beta)^{-1}[(\beta^2-\alpha^2)^5]^{-1}+(16\beta^2)^{-1}\frac{k_1{}^0(\beta)}{(\beta^2-\alpha^2)^4}\Big\}$$
$$-e^{-\alpha}\Big\{5[(\beta^2-\alpha^2)^6]^{-1}-\frac{3}{2\alpha}[(\beta^2-\alpha^2)^5]^{-1}+\frac{3}{16\alpha^2}\frac{k_1{}^0(\alpha)}{(\beta^2-\alpha^2)^4}-(96\alpha^3)^{-1}\frac{k_2{}^0(\alpha)}{(\beta^2-\alpha^2)^3}\Big\}\Big]$$

$$A(0;4,4)=\pi R^{13}\Big[e^{-\beta}\Big\{10[(\beta^2-\alpha^2)^7]^{-1}+\frac{5}{2\beta}[(\beta^2-\alpha^2)^6]^{-1}+(4\beta^2)^{-1}\frac{k_1{}^0(\beta)}{(\beta^2-\alpha^2)^5}+(96\beta^3)^{-1}\frac{k_2{}^0(\beta)}{(\beta^2-\alpha^2)^4}\Big\}$$
$$-e^{-\alpha}\Big\{10[(\beta^2-\alpha^2)^7]^{-1}-\frac{5}{2\alpha}[(\beta^2-\alpha^2)^6]^{-1}+(4\alpha^2)^{-1}\frac{k_1{}^0(\alpha)}{(\beta^2-\alpha^2)^5}-(96\alpha^3)^{-1}\frac{k_2{}^0(\alpha)}{(\beta^2-\alpha^2)^4}\Big\}\Big]$$

$$B(1;3,2)=-\pi R^6\Big[e^{-\beta}\Big\{\frac{3\beta}{2}\frac{k_1{}^0(\beta)}{(\beta^2-\alpha^2)^4}+\tfrac{1}{4}[(\beta^2-\alpha^2)^3]^{-1}\Big\}$$
$$-e^{-\alpha}\Big\{\frac{3\alpha}{2}\frac{k_1{}^0(\alpha)}{(\beta^2-\alpha^2)^4}-\tfrac{1}{2}[(\beta^2-\alpha^2)^3]^{-1}+(16\alpha)^{-1}[(\beta^2-\alpha^2)^2]^{-1}\Big\}\Big]$$

$$B(1;3,3)=-\pi R^8\Big[e^{-\beta}\Big\{3\beta\frac{k_1{}^0(\beta)}{(\beta^2-\alpha^2)^5}+\tfrac{3}{4}[(\beta^2-\alpha^2)^4]^{-1}+(16\beta)^{-1}[(\beta^2-\alpha^2)^3]^{-1}\Big\}$$
$$-e^{-\alpha}\Big\{3\alpha\frac{k_1{}^0(\alpha)}{(\beta^2-\alpha^2)^5}-\tfrac{3}{4}[(\beta^2-\alpha^2)^4]^{-1}+(16\alpha)^{-1}[(\beta^2-\alpha^2)^3]^{-1}\Big\}\Big]$$

$$B(1;4,2)=\pi R^8\Big[e^{-\beta}\Big\{2\beta\frac{k_1{}^0(\beta)}{(\beta^2-\alpha^2)^5}+\tfrac{1}{4}[(\beta^2-\alpha^2)^4]^{-1}\Big\}$$
$$-e^{-\alpha}\Big\{2\alpha\frac{k_1{}^0(\alpha)}{(\beta^2-\alpha^2)^5}-\tfrac{3}{4}[(\beta^2-\alpha^2)^4]^{-1}+(8\alpha)^{-1}[(\beta^2-\alpha^2)^3]^{-1}-(96\alpha^2)^{-1}\frac{k_1{}^0(\alpha)}{(\beta^2-\alpha^2)^2}\Big\}\Big]$$

TABLE VIII (*Continued*)

$$B(1;4,3)=\pi R^{10}\Big[e^{-\beta}\Big\{5\beta\frac{k_1^0(\beta)}{(\beta^2-\alpha^2)^6}+[(\beta^2-\alpha^2)^5]^{-1}+(16\beta)^{-1}[(\beta^2-\alpha^2)^4]^{-1}\Big\}$$
$$-e^{-\alpha}\Big\{5\alpha\frac{k_1^0(\alpha)}{(\beta^2-\alpha^2)^6}-\tfrac{3}{2}[(\beta^2-\alpha^2)^5]^{-1}+\frac{3}{16\alpha}[(\beta^2-\alpha^2)^4]^{-1}-(96\alpha^2)^{-1}\frac{k_1^0(\alpha)}{(\beta^2-\alpha^2)^3}\Big\}\Big]$$

$$B(1;4,4)=\pi R^{12}\Big[e^{-\beta}\Big\{10\beta\frac{k_1^0(\beta)}{(\beta^2-\alpha^2)^7}+\tfrac{5}{2}[(\beta^2-\alpha^2)^6]^{-1}+(4\beta)^{-1}[(\beta^2-\alpha^2)^5]^{-1}+(96\beta^2)^{-1}\frac{k_1^0(\beta)}{(\beta^2-\alpha^2)^4}\Big\}$$
$$-e^{-\alpha}\Big\{10\alpha\frac{k_1^0(\alpha)}{(\beta^2-\alpha^2)^7}-\tfrac{5}{2}[(\beta^2-\alpha^2)^6]^{-1}+(4\alpha)^{-1}[(\beta^2-\alpha^2)^5]^{-1}-(96\alpha^2)^{-1}\frac{k_1^0(\alpha)}{(\beta^2-\alpha^2)^4}\Big\}\Big]$$

$$A(2;2,2)=-\pi R^5\Big[e^{-\beta}\Big\{\frac{k_2^0(\beta)}{(\beta^2-\alpha^2)^3}+(4\beta)^{-1}\frac{k_2^1(\beta)}{(\beta^2-\alpha^2)^2}\Big\}-e^{-\alpha}\Big\{\frac{k_2^0(\alpha)}{(\beta^2-\alpha^2)^3}-(4\alpha)^{-1}\frac{k_2^1(\alpha)}{(\beta^2-\alpha^2)^2}\Big\}-\tfrac{3}{2}(\alpha^4\beta^4)^{-1}\Big]$$

$$A(2;3,2)=\pi R^7\Big[e^{-\beta}\Big\{\frac{3}{2}\frac{k_2^0(\beta)}{(\beta^2-\alpha^2)^4}+(4\beta)^{-1}\frac{k_2^1(\beta)}{(\beta^2-\alpha^2)^3}\Big\}$$
$$-e^{-\alpha}\Big\{\frac{3}{2}\frac{k_2^0(\alpha)}{(\beta^2-\alpha^2)^4}-(2\alpha)^{-1}\frac{k_2^1(\alpha)}{(\beta^2-\alpha^2)^3}+(16\alpha^2)^{-1}\frac{k_2^2(\alpha)}{(\beta^2-\alpha^2)^2}\Big\}+\tfrac{3}{2}(\alpha^6\beta^4)^{-1}\Big]$$

$$A(2;3,3)=\pi R^9\Big[e^{-\beta}\Big\{3\frac{k_2^0(\beta)}{(\beta^2-\alpha^2)^5}+\frac{3}{4\beta}\frac{k_2^1(\beta)}{(\beta^2-\alpha^2)^4}+(16\beta^2)^{-1}\frac{k_2^2(\beta)}{(\beta^2-\alpha^2)^3}\Big\}$$
$$-e^{-\alpha}\Big\{3\frac{k_2^0(\alpha)}{(\beta^2-\alpha^2)^5}-\frac{3}{4\alpha}\frac{k_2^1(\alpha)}{(\beta^2-\alpha^2)^4}+(16\alpha^2)^{-1}\frac{k_2^2(\alpha)}{(\beta^2-\alpha^2)^3}\Big\}+\tfrac{3}{2}(\alpha^6\beta^6)^{-1}\Big]$$

$$A(2;4,2)=-\pi R^9\Big[e^{-\beta}\Big\{2\frac{k_2^0(\beta)}{(\beta^2-\alpha^2)^5}+(4\beta)^{-1}\frac{k_2^1(\beta)}{(\beta^2-\alpha^2)^4}\Big\}$$
$$-e^{-\alpha}\Big\{2\frac{k_2^0(\alpha)}{(\beta^2-\alpha^2)^5}-\frac{3}{4\alpha}\frac{k_2^1(\alpha)}{(\beta^2-\alpha^2)^4}+(8\alpha^2)^{-1}\frac{k_2^2(\alpha)}{(\beta^2-\alpha^2)^3}-(96\alpha^3)^{-1}\frac{k_2^3(\alpha)}{(\beta^2-\alpha^2)^2}\Big\}-\tfrac{3}{2}(\alpha^8\beta^4)^{-1}\Big]$$

$$A(2;4,3)=-\pi R^{11}\Big[e^{-\beta}\Big\{5\frac{k_2^0(\beta)}{(\beta^2-\alpha^2)^6}+(\beta)^{-1}\frac{k_2^1(\beta)}{(\beta^2-\alpha^2)^5}+(16\beta^2)^{-1}\frac{k_2^2(\beta)}{(\beta^2-\alpha^2)^4}\Big\}$$
$$-e^{-\alpha}\Big\{5\frac{k_2^0(\alpha)}{(\beta^2-\alpha^2)^6}-\frac{3}{2\alpha}\frac{k_2^1(\alpha)}{(\beta^2-\alpha^2)^5}+\frac{3}{16\alpha^2}\frac{k_2^2(\alpha)}{(\beta^2-\alpha^2)^4}-(96\alpha^3)^{-1}\frac{k_2^3(\alpha)}{(\beta^2-\alpha^2)^3}\Big\}-\tfrac{3}{2}(\alpha^8\beta^6)^{-1}\Big]$$

$$A(2;4,4)=-\pi R^{13}\Big[e^{-\beta}\Big\{10\frac{k_2^0(\beta)}{(\beta^2-\alpha^2)^7}+\frac{5}{2\beta}\frac{k_2^1(\beta)}{(\beta^2-\alpha^2)^6}+(4\beta^2)^{-1}\frac{k_2^2(\beta)}{(\beta^2-\alpha^2)^5}+(96\beta^3)^{-1}\frac{k_2^3(\beta)}{(\beta^2-\alpha^2)^4}\Big\}$$
$$-e^{-\alpha}\Big\{10\frac{k_2^0(\alpha)}{(\beta^2-\alpha^2)^7}-\frac{5}{2\alpha}\frac{k_2^1(\alpha)}{(\beta^2-\alpha^2)^6}+(4\alpha^2)^{-1}\frac{k_2^2(\alpha)}{(\beta^2-\alpha^2)^5}-(96\alpha^3)^{-1}\frac{k_2^3(\alpha)}{(\beta^2-\alpha^2)^4}\Big\}-\tfrac{3}{2}(\alpha^8\beta^8)^{-1}\Big]$$

$$B(3;3,2)=\pi R^6\Big[e^{-\beta}\Big\{\frac{3\beta}{2}\frac{k_3^0(\beta)}{(\beta^2-\alpha^2)^4}+\frac{1}{4}\frac{k_3^1(\beta)}{(\beta^2-\alpha^2)^3}\Big\}$$
$$-e^{-\alpha}\Big\{\frac{3\alpha}{2}\frac{k_3^0(\alpha)}{(\beta^2-\alpha^2)^4}-\frac{1}{2}\frac{k_3^1(\alpha)}{(\beta^2-\alpha^2)^3}+(16\alpha)^{-1}\frac{k_3^2(\alpha)}{(\beta^2-\alpha^2)^2}\Big\}+\tfrac{15}{2}(\alpha^6\beta^4)^{-1}\Big]$$

TABLE VIII (*Continued*)

$$B(3;3,3)=\pi R^8\Big[e^{-\beta}\Big\{3\beta\frac{k_3^0(\beta)}{(\beta^2-\alpha^2)^5}+\frac{3}{4}\frac{k_3^1(\beta)}{(\beta^2-\alpha^2)^4}+(16\beta)^{-1}\frac{k_3^2(\beta)}{(\beta^2-\alpha^2)^3}\Big\}$$
$$-e^{-\alpha}\Big\{3\alpha\frac{k_3^0(\alpha)}{(\beta^2-\alpha^2)^5}-\frac{3}{4}\frac{k_3^1(\alpha)}{(\beta^2-\alpha^2)^4}+(16\alpha)^{-1}\frac{k_3^2(\alpha)}{(\beta^2-\alpha^2)^3}\Big\}+\tfrac{15}{2}(\alpha^6\beta^6)^{-1}\Big]$$

$$B(3;4,2)=-\pi R^8\Big[e^{-\beta}\Big\{2\beta\frac{k_3^0(\beta)}{(\beta^2-\alpha^2)^5}+\frac{1}{4}\frac{k_3^1(\beta)}{(\beta^2-\alpha^2)^4}\Big\}$$
$$-e^{-\alpha}\Big\{2\alpha\frac{k_3^0(\alpha)}{(\beta^2-\alpha^2)^5}-\frac{3}{4}\frac{k_3^1(\alpha)}{(\beta^2-\alpha^2)^4}+(8\alpha)^{-1}\frac{k_3^2(\alpha)}{(\beta^2-\alpha^2)^3}-(96\alpha^2)^{-1}\frac{k_3^3(\alpha)}{(\beta^2-\alpha^2)^2}\Big\}-\tfrac{15}{2}(\alpha^8\beta^4)^{-1}\Big]$$

$$B(3;4,3)=-\pi R^{10}\Big[e^{-\beta}\Big\{5\beta\frac{k_3^0(\beta)}{(\beta^2-\alpha^2)^6}+\frac{k_3^1(\beta)}{(\beta^2-\alpha^2)^5}+(16\beta)^{-1}\frac{k_3^2(\beta)}{(\beta^2-\alpha^2)^4}\Big\}$$
$$-e^{-\alpha}\Big\{5\alpha\frac{k_3^0(\alpha)}{(\beta^2-\alpha^2)^6}-\frac{3}{2}\frac{k_3^1(\alpha)}{(\beta^2-\alpha^2)^5}+\frac{3}{16\alpha}\frac{k_3^2(\alpha)}{(\beta^2-\alpha^2)^4}-(96\alpha^2)^{-1}\frac{k_3^3(\alpha)}{(\beta^2-\alpha^2)^3}\Big\}-\tfrac{15}{2}(\alpha^8\beta^6)^{-1}\Big]$$

$$B(3;4,4)=-\pi R^{12}\Big[e^{-\beta}\Big\{10\beta\frac{k_3^0(\beta)}{(\beta^2-\alpha^2)^7}+\frac{5}{2}\frac{k_3^1(\beta)}{(\beta^2-\alpha^2)^6}+(4\beta)^{-1}\frac{k_3^2(\beta)}{(\beta^2-\alpha^2)^5}+(96\beta^2)^{-1}\frac{k_3^3(\beta)}{(\beta^2-\alpha^2)^4}\Big\}$$
$$-e^{-\alpha}\Big\{10\alpha\frac{k_3^0(\alpha)}{(\beta^2-\alpha^2)^7}-\frac{5}{2}\frac{k_3^1(\alpha)}{(\beta^2-\alpha^2)^6}+(4\alpha)^{-1}\frac{k_3^2(\alpha)}{(\beta^2-\alpha^2)^5}-(96\alpha^2)^{-1}\frac{k_3^3(\alpha)}{(\beta^2-\alpha^2)^4}\Big\}-\tfrac{15}{2}(\alpha^8\beta^8)^{-1}\Big]$$

$$A(4;3,2)=-\pi R^7\Big[e^{-\beta}\Big\{\frac{3}{2}\frac{k_4^0(\beta)}{(\beta^2-\alpha^2)^4}+(4\beta)^{-1}\frac{k_4^1(\beta)}{(\beta^2-\alpha^2)^3}\Big\}$$
$$-e^{-\alpha}\Big\{\frac{3}{2}\frac{k_4^0(\alpha)}{(\beta^2-\alpha^2)^4}-(2\alpha)^{-1}\frac{k_4^1(\alpha)}{(\beta^2-\alpha^2)^3}+(16\alpha^2)^{-1}\frac{k_4^2(\alpha)}{(\beta^2-\alpha^2)^2}\Big\}$$
$$+\{-\tfrac{15}{4}(\alpha^6\beta^4)^{-1}+105(\alpha^6\beta^6)^{-1}+\tfrac{315}{2}(\alpha^8\beta^4)^{-1}\}\Big]$$

$$A(4;3,3)=-\pi R^9\Big[e^{-\beta}\Big\{3\frac{k_4^0(\beta)}{(\beta^2-\alpha^2)^5}+\frac{3}{4\beta}\frac{k_4^1(\beta)}{(\beta^2-\alpha^2)^4}+(16\beta^2)^{-1}\frac{k_4^2(\beta)}{(\beta^2-\alpha^2)^3}\Big\}$$
$$-e^{-\alpha}\Big\{3\frac{k_4^0(\alpha)}{(\beta^2-\alpha^2)^5}-\frac{3}{4\alpha}\frac{k_4^1(\alpha)}{(\beta^2-\alpha^2)^4}+(16\alpha^2)^{-1}\frac{k_4^2(\alpha)}{(\beta^2-\alpha^2)^3}\Big\}$$
$$+\{-\tfrac{15}{4}(\alpha^6\beta^6)^{-1}+\tfrac{315}{2}(\alpha^6\beta^8)^{-1}+\tfrac{315}{2}(\alpha^8\beta^6)^{-1}\}\Big]$$

$$A(4;4,2)-\pi R^9\Big[e^{-\beta}\Big\{2\frac{k_4^0(\beta)}{(\beta^2-\alpha^2)^5}+(4\beta)^{-1}\frac{k_4^1(\beta)}{(\beta^2-\alpha^2)^4}\Big\}$$
$$-e^{-\alpha}\Big\{2\frac{k_4^0(\alpha)}{(\beta^2-\alpha^2)^5}-\frac{3}{4\alpha}\frac{k_4^1(\alpha)}{(\beta^2-\alpha^2)^4}+(8\alpha^2)^{-1}\frac{k_4^2(\alpha)}{(\beta^2-\alpha^2)^3}-(96\alpha^3)^{-1}\frac{k_4^3(\alpha)}{(\beta^2-\alpha^2)^2}\Big\}$$
$$+\{\tfrac{15}{4}(\alpha^8\beta^4)^{-1}-105(\alpha^8\beta^6)^{-1}-210(\alpha^{10}\beta^4)^{-1}\}\Big]$$

TABLE VIII (*Continued*)

$$A(4;4,3)=\pi R^{11}\Bigg[e^{-\beta}\left\{5\frac{k_4{}^0(\beta)}{(\beta^2-\alpha^2)^6}+(\beta)^{-1}\frac{k_4{}^1(\beta)}{(\beta^2-\alpha^2)^5}+(16\beta^2)^{-1}\frac{k_4{}^2(\beta)}{(\beta^2-\alpha^2)^4}\right\}$$
$$-e^{-\alpha}\left\{5\frac{k_4{}^0(\alpha)}{(\beta^2-\alpha^2)^6}-\frac{3}{2\alpha}\frac{k_4{}^1(\alpha)}{(\beta^2-\alpha^2)^5}+\frac{3}{16\alpha^2}\frac{k_4{}^2(\alpha)}{(\beta^2-\alpha^2)^4}-(96\alpha^3)^{-1}\frac{k_4{}^3(\alpha)}{(\beta^2-\alpha^2)^3}\right\}$$
$$+\{\tfrac{15}{4}(\alpha^8\beta^6)^{-1}-\tfrac{315}{2}(\alpha^8\beta^8)^{-1}-210(\alpha^{10}\beta^6)^{-1}\}\Bigg]$$

$$A(4;4,4)=\pi R^{13}\Bigg[e^{-\beta}\left\{10\frac{k_4{}^0(\beta)}{(\beta^2-\alpha^2)^7}+\frac{5}{2\beta}\frac{k_4{}^1(\beta)}{(\beta^2-\alpha^2)^6}+(4\beta^2)^{-1}\frac{k_4{}^2(\beta)}{(\beta^2-\alpha^2)^5}+(96\beta^3)^{-1}\frac{k_4{}^3(\beta)}{(\beta^2-\alpha^2)^4}\right\}$$
$$-e^{-\alpha}\left\{10\frac{k_4{}^0(\alpha)}{(\beta^2-\alpha^2)^7}-\frac{5}{2\alpha}\frac{k_4{}^1(\alpha)}{(\beta^2-\alpha^2)^6}+(4\alpha^2)^{-1}\frac{k_4{}^2(\alpha)}{(\beta^2-\alpha^2)^5}-(96\alpha^3)^{-1}\frac{k_4{}^3(\alpha)}{(\beta^2-\alpha^2)^4}\right\}$$
$$+\{\tfrac{15}{4}(\alpha^8\beta^8)^{-1}-210(\alpha^8\beta^{10})^{-1}-210(\alpha^{10}\beta^8)^{-1}\}\Bigg]$$

$$B(5;3,3)=-\pi R^{8}\Bigg[e^{-\beta}\left\{3\beta\frac{k_5{}^0(\beta)}{(\beta^2-\alpha^2)^5}+\frac{3}{4}\frac{k_5{}^1(\beta)}{(\beta^2-\alpha^2)^4}+(16\beta)^{-1}\frac{k_5{}^2(\beta)}{(\beta^2-\alpha^2)^3}\right\}$$
$$-e^{-\alpha}\left\{3\alpha\frac{k_5{}^0(\alpha)}{(\beta^2-\alpha^2)^5}-\frac{3}{4}\frac{k_5{}^1(\alpha)}{(\beta^2-\alpha^2)^4}+(16\alpha)^{-1}\frac{k_5{}^2(\alpha)}{(\beta^2-\alpha^2)^3}\right\}$$
$$-\{\tfrac{105}{4}(\alpha^6\beta^6)^{-1}-\tfrac{2835}{2}(\alpha^8\beta^6)^{-1}-\tfrac{2835}{2}(\alpha^6\beta^8)^{-1}\}\Bigg]$$

$$B(5;4,3)=\pi R^{10}\Bigg[e^{-\beta}\left\{5\beta\frac{k_5{}^0(\beta)}{(\beta^2-\alpha^2)^6}+\frac{k_5{}^1(\beta)}{(\beta^2-\alpha^2)^5}+(16\beta)^{-1}\frac{k_5{}^2(\beta)}{(\beta^2-\alpha^2)^4}\right\}$$
$$-e^{-\alpha}\left\{5\alpha\frac{k_5{}^0(\alpha)}{(\beta^2-\alpha^2)^6}-\frac{3}{2}\frac{k_5{}^1(\alpha)}{(\beta^2-\alpha^2)^5}+\frac{3}{16\alpha}\frac{k_5{}^2(\alpha)}{(\beta^2-\alpha^2)^4}-(96\alpha^2)^{-1}\frac{k_5{}^3(\alpha)}{(\beta^2-\alpha^2)^3}\right\}$$
$$+\{\tfrac{105}{4}(\alpha^8\beta^6)^{-1}-\tfrac{5670}{3}(\alpha^{10}\beta^6)^{-1}-\tfrac{2835}{2}(\alpha^8\beta^8)^{-1}\}\Bigg]$$

$$B(5;4,4)=\pi R^{12}\Bigg[e^{-\beta}\left\{10\beta\frac{k_5{}^0(\beta)}{(\beta^2-\alpha^2)^7}+\frac{5}{2}\frac{k_5{}^1(\beta)}{(\beta^2-\alpha^2)^6}+(4\beta)^{-1}\frac{k_5{}^2(\beta)}{(\beta^2-\alpha^2)^5}+(96\beta^2)^{-1}\frac{k_5{}^3(\beta)}{(\beta^2-\alpha^2)^4}\right\}$$
$$-e^{-\alpha}\left\{10\alpha\frac{k_5{}^0(\alpha)}{(\beta^2-\alpha^2)^7}-\frac{5}{2}\frac{k_5{}^1(\alpha)}{(\beta^2-\alpha^2)^6}+(4\alpha)^{-1}\frac{k_5{}^2(\alpha)}{(\beta^2-\alpha^2)^5}-(96\alpha^2)^{-1}\frac{k_5{}^3(\alpha)}{(\beta^2-\alpha^2)^4}\right\}$$
$$+\{\tfrac{105}{4}(\alpha^8\beta^8)^{-1}-1890(\alpha^{10}\beta^8)^{-1}-1890(\alpha^8\beta^{10})^{-1}\}\Bigg]$$

$$A(6;3,3)=\pi R^{9}\Bigg[e^{-\beta}\left\{3\frac{k_6{}^0(\beta)}{(\beta^2-\alpha^2)^5}+\frac{3}{4\beta}\frac{k_6{}^1(\beta)}{(\beta^2-\alpha^2)^4}+(16\beta^2)^{-1}\frac{k_6{}^2(\beta)}{(\beta^2-\alpha^2)^3}\right\}$$
$$-e^{-\alpha}\left\{3\frac{k_6{}^0(\alpha)}{(\beta^2-\alpha^2)^5}-\frac{3}{4\alpha}\frac{k_6{}^1(\alpha)}{(\beta^2-\alpha^2)^4}+(16\alpha^2)^{-1}\frac{k_6{}^2(\alpha)}{(\beta^2-\alpha^2)^3}\right\}$$
$$+\{\tfrac{105}{16}(\alpha^6\beta^6)^{-1}-\tfrac{2835}{4}(\alpha^8\beta^6)^{-1}-\tfrac{2835}{4}(\alpha^6\beta^8)^{-1}\}+\left\{\frac{10935}{2}\left(\frac{6}{\alpha^{10}\beta^6}+\frac{9}{\alpha^8\beta^8}+\frac{6}{\alpha^6\beta^{10}}\right)\right\}\Bigg]$$

TABLE VIII (*Continued*)

$$A(6;4,3)=-\pi R^{11}\Bigg[e^{-\beta}\Bigg\{5\frac{k_6{}^0(\beta)}{(\beta^2-\alpha^2)^6}+(\beta)^{-1}\frac{k_6{}^1(\beta)}{(\beta^2-\alpha^2)^5}+(16\beta^2)^{-1}\frac{k_6{}^2(\beta)}{(\beta^2-\alpha^2)^4}\Bigg\}$$
$$-e^{-\alpha}\Bigg\{5\frac{k_6{}^0(\alpha)}{(\beta^2-\alpha^2)^6}-\frac{3}{2\alpha}\frac{k_6{}^1(\alpha)}{(\beta^2-\alpha^2)^5}+\frac{3}{16\alpha^2}\frac{k_6{}^2(\alpha)}{(\beta^2-\alpha^2)^4}-(96\alpha^3)^{-1}\frac{k_6{}^3(\alpha)}{(\beta^2-\alpha^2)^3}\Bigg\}$$
$$-\{\tfrac{105}{16}(\alpha^8\beta^6)^{-1}-\tfrac{2835}{3}(\alpha^{10}\beta^6)^{-1}-\tfrac{2835}{4}(\alpha^8\beta^8)^{-1}\}-\Bigg\{\frac{10935}{2}\Bigg(\frac{10}{\alpha^{12}\beta^6}+\frac{12}{\alpha^{10}\beta^8}+\frac{6}{\alpha^8\beta^{10}}\Bigg)\Bigg\}\Bigg]$$

$$A(6;4,4)=-\pi R^{13}\Bigg[e^{-\beta}\Bigg\{10\frac{k_6{}^0(\beta)}{(\beta^2-\alpha^2)^7}+\frac{5}{2\beta}\frac{k_6{}^1(\beta)}{(\beta^2-\alpha^2)^6}+(4\beta^2)^{-1}\frac{k_6{}^2(\beta)}{(\beta^2-\alpha^2)^5}+(96\beta^3)^{-1}\frac{k_6{}^3(\beta)}{(\beta^2-\alpha^2)^4}\Bigg\}$$
$$-e^{-\alpha}\Bigg\{10\frac{k_6{}^0(\alpha)}{(\beta^2-\alpha^2)^7}-\frac{5}{2\alpha}\frac{k_6{}^1(\alpha)}{(\beta^2-\alpha^2)^6}+(4\alpha^2)^{-1}\frac{k_6{}^2(\alpha)}{(\beta^2-\alpha^2)^5}-(96\alpha^3)^{-1}\frac{k_6{}^3(\alpha)}{(\beta^2-\alpha^2)^4}\Bigg\}$$
$$-\{\tfrac{105}{16}(\alpha^8\beta^8)^{-1}-945(\alpha^{10}\beta^8)^{-1}-945(\alpha^8\beta^{10})^{-1}\}-10935\Bigg\{\frac{5}{\alpha^{12}\beta^8}+\frac{8}{\alpha^{10}\beta^{10}}+\frac{5}{\alpha^8\beta^{12}}\Bigg\}\Bigg]$$

[a] To obtain $A(2m;q,p)$ from $A(2m;p,q)$ and $B(2m+1;q,p)$ from $B(2m+1;p,q)$ interchange α and β. ($\alpha\to\beta$; $\beta\to\alpha$).

and

$$B(2m+1;p+1,q+1)=(-\tfrac{1}{2}R^2)^{p+q}[p!q!]^{-1}$$
$$[\alpha^{-1}(\partial/\partial\alpha)]^p[\beta^{-1}(\partial/\partial\beta)]^qB(2m+1;1,1),\quad(19)$$

where in Eqs. (18) and (19), $\alpha=p_aR$ and $\beta=p_bR$.

For the evaluation of $A(2m;1,1)$ and $B(2m+1;1,1)$ it is useful to define one further auxiliary function

$$F_n(\gamma)=\int_0^1(1-y^2)^n\exp(-\gamma y)\,dy,\quad(20)$$

which has the differential recursion relation

$$(\partial/\partial\gamma)F_n(\gamma)=\tfrac{1}{2}(n+1)^{-1}[\gamma F_{n+1}(\gamma)-1].\quad(21)$$

From Appendix A, the following analytical expression can be derived for $F_n(\gamma)$

$$F_n(\gamma)=\sum_{k=0}^{n}(-1)^k\binom{n}{k}(2k)!\gamma^{-2k-1}$$
$$-(-1)^n2^nn!\gamma^{-n}(2/\pi\gamma)^{\frac{1}{2}}K_{n+\frac{1}{2}}(\gamma),\quad(22)$$

where $K_{n+\frac{1}{2}}(\gamma)$ in Eq. (22) is the hyperbolic Bessel function[17] of half integral order. Table IV lists the explicit expressions for $F_n(\gamma)$ ($n=0,1,2,\cdots,7$) that are needed in the evaluation of $A(2m;1,1)$ and $B(2m+1;1,1)$.

As derived in Appendix B, the primitives $A(2m;1,1)$ and $B(2m+1;1,1)$ can be expressed in terms of the $F_n(\gamma)$ functions defined in Eq. (20):

$$A(2m;1,1)=(-1)^m\pi R2^{-2m-1}[(2m)!]^{-1}(\beta^2-\alpha^2)^{-1}$$
$$\times\{\beta^{2m+1}F_{2m}(\beta)-\alpha^{2m+1}F_{2m}(\alpha)\},\quad(23a)$$

and

$$B(2m+1;1,1)=(-1)^{m+1}\pi2^{-2m-2}[(2m+1)!]^{-1}$$
$$\times(\beta^2-\alpha^2)^{-1}\{\beta^{2m+3}F_{2m+1}(\beta)-\alpha^{2m+3}F_{2m+1}(\alpha)\},\quad(23b)$$

for the case of different effective nuclear charges $p_a\neq p_b$ (and therefore $\alpha\neq\beta$) and

$$A(2m;1,1)=(-1)^m\pi R2^{-2m-3}[(2m+1)!]^{-1}\gamma2^{m-1}$$
$$\times\{\gamma^2F_{2m+1}(\gamma)+2(2m+1)^2F_{2m}(\gamma)-\gamma\}\quad(24a)$$

and

$$B(2m+1;1,1)=(-1)^{m+1}\pi2^{-2m-4}[(2m+2)!]^{-1}$$
$$\times\gamma^{2m+1}\{\gamma^2F_{2m+2}(\gamma)+2(2m+2)(2m+3)F_{2m+1}(\gamma)-\gamma\}\quad(24b)$$

for the case of identical effective nuclear charges $p_a=p_b$ (and therefore $\alpha=\beta\equiv\gamma$). Table V gives the explicit expressions for $A(2m;1,1)$, ($m=0,1,2$, and 3), and $B(2m+1;1,1)$, ($m=0,1,2$) in terms of the $F_n(\gamma)$ functions as derivable from Eq. (23) for the case of unequal nuclear charges and Table VI gives the corresponding expressions derivable from Eqs. (24) for equal nuclear charges.

A final simplification of the resulting formulas is achieved if we define the following polynomials in $1/\gamma$

$$k_n{}^0(\gamma)=(\pi/2\gamma)^{-\frac{1}{2}}e^{\gamma}K_{n+\frac{1}{2}}(\gamma)=\sum_{m=0}^{n}\frac{(n+m)!}{m!(n-m)!}(2\gamma)^{-m},\quad(25)$$

and

$$k_{2n}{}^p(\gamma)=\gamma^{p-1}[1-(\partial/\partial\gamma)]\gamma^{1-p}k_{2n}{}^{p-1}(\gamma);\quad(26a)$$

TABLE IX. $A(2m;\,p,\,q)$ and $B(2m+1;\,p,\,q)$ in terms of $k_m{}^p(\gamma)$ case of equal nuclear charges ($\alpha=\beta$).[a]

$$A(0;3,2)=(4!2^5)^{-1}\pi R^7\gamma^{-4}k_3{}^0(\gamma)e^{-\gamma}$$

$$A(0;3,3)=A(0;4,2)=(5!2^6)^{-1}\pi R^9\gamma^{-5}k_4{}^0(\gamma)e^{-\gamma}$$

$$A(0;4,3)=(6!2^7)^{-1}\pi R^{11}\gamma^{-6}k_5{}^0(\gamma)e^{-\gamma}$$

$$A(0;4,4)=(7!2^8)^{-1}\pi R^{13}\gamma^{-7}k_6{}^0(\gamma)e^{-\gamma}$$

$$B(1;3,2)=(4!2^5)^{-1}\pi R^6\gamma^{-3}k_2{}^0(\gamma)e^{-\gamma}$$

$$B(1;3,3)=B(1;4,2)=(5!2^6)^{-1}\pi R^8\gamma^{-4}k_3{}^0(\gamma)e^{-\gamma}$$

$$B(1;4,3)=(6!2^7)^{-1}\pi R^{10}\gamma^{-5}k_4{}^0(\gamma)e^{-\gamma}$$

$$B(1;4,4)=(7!2^8)^{-1}\pi R^{12}\gamma^{-6}k_5{}^0(\gamma)e^{-\gamma}$$

$$A(2;2,2)=-\pi R^5[(3!2^4)^{-1}\gamma^{-3}k_2{}^3(\gamma)e^{-\gamma}-(3/2)\gamma^{-8}]$$

$$A(2;3,2)=-\pi R^7[(4!2^5)^{-1}\gamma^{-4}k_2{}^4(\gamma)e^{-\gamma}-(3/2)\gamma^{-10}]$$

$$A(2;3,3)=A(2;4,2)=-\pi R^9[(5!2^6)^{-1}\gamma^{-5}k_2{}^5(\gamma)e^{-\gamma}-(3/2)\gamma^{-12}]$$

$$A(2;4,3)=-\pi R^{11}[(6!2^7)^{-1}\gamma^{-6}k_2{}^6(\gamma)e^{-\gamma}-(3/2)\gamma^{-14}]$$

$$A(2;4,4)=-\pi R^{13}[(7!2^8)^{-1}\gamma^{-7}k_2{}^7(\gamma)e^{-\gamma}-(3/2)\gamma^{-16}]$$

$$B(3;3,2)=-\pi R^6[(4!2^5)^{-1}\gamma^{-3}k_3{}^4(\gamma)e^{-\gamma}-(15/2)\gamma^{-10}]$$

$$B(3;3,3)=B(3;4,2)=-\pi R^8[(5!2^6)^{-1}\gamma^{-4}k_3{}^5(\gamma)e^{-\gamma}-(15/2)\gamma^{-12}]$$

$$B(3;4,3)=-\pi R^{10}[(6!2^7)^{-1}\gamma^{-5}k_3{}^6(\gamma)e^{-\gamma}-(15/2)\gamma^{-14}]$$

$$B(3;4,4)=-\pi R^{12}[(7!2^8)^{-1}\gamma^{-6}k_3{}^7(\gamma)e^{-\gamma}-(15/2)\gamma^{-16}]$$

$$A(4;3,2)=\pi R^7[(4!2^5)^{-1}\gamma^{-4}k_4{}^4(\gamma)e^{-\gamma}+(15/4)\gamma^{-10}-(525/2)\gamma^{-12}]$$

$$A(4;3,3)=A(4;4,2)=\pi R^9[(5!2^6)^{-1}\gamma^{-5}k_4{}^5(\gamma)e^{-\gamma}+(15/4)\gamma^{-12}-315\gamma^{-14}]$$

$$A(4;4,3)=\pi R^{11}[(6!2^7)^{-1}\gamma^{-6}k_4{}^6(\gamma)e^{-\gamma}+(15/4)\gamma^{-14}-(735/2)\gamma^{-16}]$$

$$A(4;4,4)=\pi R^{13}[(7!2^8)^{-1}\gamma^{-7}k_4{}^7(\gamma)e^{-\gamma}+(15/4)\gamma^{-16}-420\gamma^{-18}]$$

$$B(5;3,3)=\pi R^8[(5!2^6)^{-1}\gamma^{-4}k_5{}^5(\gamma)e^{-\gamma}+(105/4)\gamma^{-12}-2835\gamma^{-14}]$$

$$B(5;4,3)=\pi R^{10}[(6!2^7)^{-1}\gamma^{-5}k_5{}^6(\gamma)e^{-\gamma}+(105/4)\gamma^{-14}-(6615/2)\gamma^{-16}]$$

$$B(5;4,4)=\pi R^{12}[(7!2^8)^{-1}\gamma^{-6}k_5{}^7(\gamma)e^{-\gamma}+(105/4)\gamma^{-16}-3780\gamma^{-18}]$$

$$A(6;3,3)=-\pi R^9[(5!2^6)^{-1}\gamma^{-5}k_6{}^5(\gamma)e^{-\gamma}-(105/16)\gamma^{-12}+(2835/2)\gamma^{-14}-(218\,295/2)\gamma^{-16}]$$

$$A(6;4,3)=-\pi R^{11}[(6!2^7)^{-1}\gamma^{-6}k_6{}^6(\gamma)e^{-\gamma}-(105/16)\gamma^{-14}+(6615/4)\gamma^{-16}-145\,530\gamma^{-18}]$$

$$A(6;4,4)=-\pi R^{13}[(7!2^8)^{-1}\gamma^{-7}k_6{}^7(\gamma)e^{-\gamma}-(105/16)\gamma^{-16}+1890\gamma^{-18}-187\,110\gamma^{-20}]$$

[a] Since $\alpha=\beta=\gamma$, the following identities hold: $A(2m;\,p,\,q)=A(2m;\,q,\,p)$ and $B(2m+1,\,p,\,q)=B(2m+1,\,q,\,p)$.

and

$$k_{2n+1}{}^p(\gamma)=\gamma^{p-2}[1-(\partial/\partial\gamma)]\gamma^{2-p}k_{2n+1}{}^{p-1}(\gamma). \quad (26b)$$

Table VII is a partial collection of some of the $k_m{}^p(\gamma)$ needed in this study. This table contains all the polynomials needed for the case of unequal nuclear charges. For the case of identical nuclear charges, higher p values are needed but are not listed due to the cumbersome coefficients, though these can easily be obtained from Eqs. (26).

The extensive tabulation of all the $A(2m;\,p,\,q)$ and $B(2m+1;\,p,\,q)$ needed for integrals I_1 and I_2 of Eqs. (7) as shown in Tables II and III is presented in Table VIII for the case of different nuclear charges

TABLE X. One-center integrals I_1 and $I_2(R=0)$—different nuclear charges.

$$[1S_a \mid 1 \mid 3D\Sigma_a] = (1/180)p_a^4p_b^3(p_a+p_b)^{-4} + (1/45)p_a^4p_b^4(p_a+p_b)^{-5}$$
$$[2S_a \mid 1 \mid 3D\Sigma_a] = (1/180)p_a^4p_b^3(p_a+p_b)^{-4} + (1/45)p_a^4p_b^4(p_a+p_b)^{-5} - (1/27)p_a^4p_b^5(p_a+p_b)^{-6}$$
$$[3S_a \mid 1 \mid 3D\Sigma_a] = (1/180)p_a^5p_b^3(p_a+p_b)^{-5} + (1/36)p_a^5p_b^4(p_a+p_b)^{-6} - (1/18)p_a^5p_b^5(p_a+p_b)^{-7}$$
$$[2P\Sigma_a \mid 1 \mid 2P\Sigma_a] = (1/15)p_a^4p_b^4(p_a+p_b)^{-5}$$
$$[2P\Sigma_a \mid 1 \mid 3P\Sigma_a] = (1/15)p_a^4p_b^5(p_a+p_b)^{-6}$$
$$[3P\Sigma_a \mid 1 \mid 3P\Sigma_a] = (2/25)p_a^5p_b^5(p_a+p_b)^{-7}$$
$$[3D\Sigma_a \mid 1 \mid 3D\Sigma_a] = -(2/189)p_a^5p_b^5(p_a+p_b)^{-7}$$
$$[2P\Pi_a \mid 1 \mid 2P\Pi_a] = [2P\bar{\Pi}_a \mid 1 \mid 2P\bar{\Pi}_a] = -(1/30)p_a^4p_b^4(p_a+p_b)^{-5}$$
$$[2P\Pi_a \mid 1 \mid 3P\Pi_a] = [2P\bar{\Pi}_a \mid 1 \mid 3P\bar{\Pi}_a] = -(1/30)p_a^4p_b^5(p_a+p_b)^{-6}$$
$$[3P\Pi_a \mid 1 \mid 3P\Pi_a] = [3P\bar{\Pi}_a \mid 1 \mid 3P\bar{\Pi}_a] = -(1/25)p_a^5p_b^5(p_a+p_b)^{-7}$$
$$[3D\Pi_a \mid 1 \mid 3D\Pi_a] = [3D\bar{\Pi}_a \mid 1 \mid 3D\bar{\Pi}_a] = -(1/189)p_a^5p_b^5(p_a+p_b)^{-7}$$
$$[3D\Delta_a \mid 1 \mid 3D\Delta_a] = [3D\bar{\Delta}_a \mid 1 \mid 3D\bar{\Delta}_a] = (2/189)p_a^5p_b^5(p_a+p_b)^{-7}$$
$$[1S_a \mid 2 \mid 3D\Delta_a] = (2/45)\sqrt{3}p_a^4p_b^4(p_a+p_b)^{-5} + (1/90)\sqrt{3}p_a^4p_b^3(p_a+p_b)^{-4}$$
$$[2S_a \mid 2 \mid 3D\Delta_a] = (1/90)\sqrt{3}p_a^4p_b^3(p_a+p_b)^{-4} + (2/45)\sqrt{3}p_a^4p_b^4(p_a+p_b)^{-5} - (2/27)\sqrt{3}p_a^4p_b^5(p_a+p_b)^{-6}$$
$$[3S_a \mid 2 \mid 3D\Delta_a] = (1/90)\sqrt{3}p_a^5p_b^3(p_a+p_b)^{-5} + (1/18)\sqrt{3}p_a^5p_b^4(p_a+p_b)^{-6} - (1/9)\sqrt{3}p_a^5p_b^5(p_a+p_b)^{-7}$$
$$[2P\Pi_a \mid 2 \mid 2P\Pi_a] = -[2P\bar{\Pi}_a \mid 2 \mid 2P\bar{\Pi}_a] = (1/5)p_a^4p_b^4(p_a+p_b)^{-5}$$
$$[2P\Pi_a \mid 2 \mid 3P\Pi_a] = -[2P\bar{\Pi}_a \mid 2 \mid 3P\bar{\Pi}_a] = (1/5)p_a^4p_b^5(p_a+p_b)^{-6}$$
$$[3P\Pi_a \mid 2 \mid 3P\Pi_a] = -[3P\bar{\Pi}_a \mid 2 \mid 3P\bar{\Pi}_a] = (6/25)p_a^5p_b^5(p_a+p_b)^{-7}$$
$$[3D\Pi_a \mid 2 \mid 3D\Pi_a] = -[3D\bar{\Pi}_a \mid 2 \mid 3D\bar{\Pi}_a] = -(2/63)p_a^5p_b^5(p_a+p_b)^{-7}$$
$$[3D\Sigma_a \mid 2 \mid 3D\Delta_a] = (4/189)\sqrt{3}p_a^5p_b^5(p_a+p_b)^{-7}$$

and in Table IX for the case of equal nuclear charges in terms of the polynomials $k_m^p(\gamma)$ defined by Eqs. (25) and (26) and tabulated in Table VII.

V. ONE-CENTER RESULTS

For the one-center case, we have, from the properties of spherical Bessel functions,

$$j_p(0) = \delta_{p,0}, \tag{27}$$

so that the only terms contributing to the one-center result are those in which the terms $A(0;\, p,\, q)$ arise. This is equivalent to the additional selection rule $|L+L'| = 2,\ 4$. The final results for the one-center case with different nuclear charges are presented in Table X and for the case of equal nuclear charges in Table XI.

APPENDIX A: EVALUATION OF $F_n(\gamma)$

From Eq. (20) of the text, $F_n(\gamma)$ is given by

$$F_n(\gamma) = \int_0^1 (1-y^2)^n e^{-\gamma y} dy. \tag{A1}$$

This integral is equal to

$$F_n(\gamma) = \int_0^\infty (1-y^2)^n e^{-\gamma y} dy - \int_1^\infty (1-y^2)^n e^{-\gamma y} dy. \tag{A2}$$

For the first term in (A2), after expanding $(1-y^2)^n$ by the binomial expansion and integrating termwise, we obtain

$$\int_0^\infty (1-y^2)^n e^{-\gamma y} dy = \sum_{k=0}^n (-1)^k \binom{n}{k} \int_0^\infty y^{2k} e^{-\gamma y} dy,$$
$$= \sum_{k=0}^n (-1)^k \binom{n}{k} (2k)!\gamma^{-2k-1}. \tag{A3}$$

For the second term in (A2), noting that an integral representation of the hyperbolic Bessel function $K_{n+\frac{1}{2}}$ is

$$K_{n+\frac{1}{2}}(Z) = (\tfrac{1}{2}Z)^{n+\frac{1}{2}} \pi^{\frac{1}{2}} (n!)^{-1} \int_1^\infty e^{-yz} (y^2-1)^n dy, \tag{A4}$$

we finally obtain

$$\int_1^\infty (1-y^2)^n e^{-\gamma y} dy = (-1)^n 2^n n! \gamma^{-n} \left(\frac{2}{\pi\gamma}\right)^{\frac{1}{2}} K_{n+\frac{1}{2}}(\gamma). \tag{A5}$$

TABLE XI. One-center integrals I_1 and I_2 ($R=0$)—equal nuclear charges.[a]

$$[1S_a \mid 1 \mid 3D\Sigma_a] = (1/960)p^3$$
$$[2S_a \mid 1 \mid 3D\Sigma_a] = (1/2160)p^3$$
$$[3S_a \mid 1 \mid 3D\Sigma_a] = (1/5760)p^3$$
$$[2P\Sigma_a \mid 1 \mid 2P\Sigma_a] = (1/480)p^3$$
$$[2P\Sigma_a \mid 1 \mid 3P\Sigma_a] = (1/960)p^3$$
$$[3P\Sigma_a \mid 1 \mid 3P\Sigma_a] = (1/1600)p^3$$
$$[3D\Sigma_a \mid 1 \mid 3D\Sigma_a] = -(1/12\,096)p^3$$
$$[2P\Pi_a \mid 1 \mid 2P\Pi_a] = [2P\bar{\Pi}_a \mid 1 \mid 2P\bar{\Pi}_a] = -(1/960)p^3$$
$$[2P\Pi_a \mid 1 \mid 3P\Pi_a] = [2P\bar{\Pi}_a \mid 1 \mid 3P\bar{\Pi}_a] = -(1/1920)p^3$$
$$[3P\Pi_a \mid 1 \mid 3P\Pi_a] = [3P\bar{\Pi}_a \mid 1 \mid 3P\bar{\Pi}_a] = -(1/3200)p^3$$
$$[3D\Pi_a \mid 1 \mid 3D\Pi_a] = [3D\bar{\Pi}_a \mid 1 \mid 3D\bar{\Pi}_a] = -(1/24\,192)p^3$$
$$[3D\Delta_a \mid 1 \mid 3D\Delta_a] = [3D\bar{\Delta}_a \mid 1 \mid 3D\bar{\Delta}_a] = (1/12\,096)p^3$$
$$[1S_a \mid 2 \mid 3D\Delta_a] = (1/480)\sqrt{3}p^3$$
$$[2S_a \mid 2 \mid 3D\Delta_a] = (1/1080)\sqrt{3}p^3$$
$$[3S_a \mid 2 \mid 3D\Delta_a] = (1/2880)\sqrt{3}p^3$$
$$[2P\Pi_a \mid 2 \mid 2P\Pi_a] = -[2P\bar{\Pi}_a \mid 2 \mid 2P\bar{\Pi}_a] = (1/160)p^3$$
$$[2P\Pi_a \mid 2 \mid 3P\Pi_a] = -[2P\bar{\Pi}_a \mid 2 \mid 3P\bar{\Pi}_a] = (1/320)p^3$$
$$[3P\Pi_a \mid 2 \mid 3P\Pi_a] = -[3P\bar{\Pi}_a \mid 2 \mid 3P\bar{\Pi}_a] = (3/1600)p^3$$
$$[3D\Pi_a \mid 2 \mid 3D\Pi_a] = -[3D\bar{\Pi}_a \mid 2 \mid 3D\bar{\Pi}_a] = -(1/4032)p^3$$
$$[3D\Sigma_a \mid 2 \mid 3D\Delta_a] = (1/6048)\sqrt{3}p^3$$

[a] The nuclear charges p_a and p_b are equal to p. ($p_a = p_b = p$.)

Thus, taking the difference of (A3) and (A5), we have Eq. (22) of the text.[18]

APPENDIX B: DERIVATION OF $A(2m;\,1,\,1)$ AND $B(2m+1;\,1,\,1)$ IN TERMS OF THE $F_n(\gamma)$

Equation (16) of the text, when $p=q=1$, is given by

$$A(2m;\,1,\,1) = \int_0^\infty \frac{k^2 j_{2m}(kR)\,dk}{(k^2+p_a^2)(k^2+p_b^2)}. \quad \text{(B1)}$$

Using the integral representation of $j_p(x)$,[17]

$$j_p(x) = [p!]^{-1}(x/2)^p \int_0^1 (1-y^2)^p \cos xy\,dy. \quad \text{(B2)}$$

In Eq. (B1), inverting the order of integration, and integrating over k, noting that

$$\int_0^\infty \frac{k^{2m+2}\cos kRy\,dk}{(k^2+p_a^2)(k^2+p_b^2)} = (-1)^m(\tfrac{1}{2}\pi)(p_b^2-p_a^2)^{-1} \times\{p_b^{2m+1}\exp(-p_bRy) - p_a^{2m+1}\exp(-p_aRy)\}, \quad \text{(B3)}$$

we have

$$A(2m;\,1,\,1) = (-1)^m \pi R 2^{-2m-1}[(2m)!]^{-1}(\beta^2-\alpha^2)^{-1} \times\int_0^\infty (1-y^2)^{2m}\{\beta^{2m+1}e^{-\beta y} - \alpha^{2m+1}e^{-\alpha y}\}\,dy, \quad \text{(B4)}$$

where in Eq. (B4) we have replaced p_bR by β and p_aR by α. Using the definition of $F_n(\gamma)$ as given by Eq. (20) of the text, Eq. (23a) is immediately obtained. A similar application of the integral representation Eq. (B2) for $j_{2m+1}(kR)$, followed by inverting the order of integration and using Eq. (B3) appropriately leads to the result quoted in Eq. (23b) for $B(2m+1;\,1,\,1)$.

Equations (24a) and (24b) of the text follow in a straightforward manner by choosing $p_aR = p_bR \equiv \gamma$, using Eq. (B2) and the analog of Eq. (B3) in the case when $p_a = p_b$

$$\int_0^\infty \frac{k^{2m+2}\cos kRy\,dy}{(k^2+p_a^2)^2} = (-1)^m(\tfrac{1}{4}\pi)\{2m+1-\alpha y\}p_a^{2m-1}e^{-\alpha y}. \quad \text{(B5)}$$

[18] The author is indebted to S. Boorstein for this simplified derivation.